STEADY AND UNSTEADY STATE DISPERSION OF AIR POLLUTANTS: EFFECTS OF REMOVAL MECHANISMS

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Dedicated to My Parents

Sri Banbari Singh Chauhan

Smt. Munni Devi

CERTIFICATE

This is to certify that the matter embodied in the thesis entitled "STEADY AND UNSTEADY DISPERSION OF AIR POLLUTANTS :EFFECTS OF REMOVAL MECHANISMS" by Mr. Runchhor Singh Chauhan for the award of Degree of Doctor of Philosophy of the Indian Institute of Technology, Kanpur is a record of bonafide research work carried out by him under our supervision and guidance. The results embodied in this thesis have not been submitted to any other University or Institute for the award of any degree and diploma.

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CONTENTS

CHAPTER I

GENERAL INTRODUCTION

1.1 INTRODUCTION

"The term air pollution may be defined as any undesirable addition to our environment in the form of dust, particulate matter, fume, gas, mist, smoke, smog etc., for duration and in such quantities that it becomes harmful to human, animal and plant life, to our living, to our enjoyment and to our property". Air pollutants (compounds of sulfur, carbon, nitrogen, etc.) which are emitted from industrial and other man made sources affect the ecosystems in general and its specific components in particular in several ways leading to harmful consequences. It affects our health, our living, our property, our priceless monuments etc. It also harms animal and plant species and damages the ecosystem creating various kinds of problems in the form of diseases, epidemics, climate changes, etc.

It is, therefore, absolutely essential to study the dispersion of pollutants, emitted by various industries and man-made projects, required for environmental assessment programme of polluted regions on one hand and to determine its impact on both living and nonliving species on the other.

In view of this, in this thesis the following type of problems are investigated

(i) Unsteady state dispersion of reactive air pollutant forming secondary pollutant in the atmosphere with various kinds of removal mechanisms including deposition on the ground

(ii) Steady state dispersion of reactive pollutant with variable wind velocity and diffusivities from point and line sources by considering deposition on the ground.

(iii) Steady and unsteady state dispersion of air pollutants in presence of green belt.

In the following we present an outline of the relevant literature so that the work done in the thesis can be seen in its proper perspective.

1.2 OUTLINE OF RELEVANT LITERATURE

In the study of pollutant dispersion, we are generally interested in finding out the concentration of a pollutant, after being emitted into atmosphere, at a specified location and time, which depends upon the number of sources, their locations, emission rates, etc. The dispersal process is governed by the process of molecular diffusion and convection and depends upon meteorological factors such as wind, temperature inversion, topography of terrain, removal mechanisms such as dry deposition, rainout/washout, etc. (Calder, 1961; Pasquill, 1962; Turner, 1970; Carpenter et al., 1971; Heines and Peters, 1973a, 1973b; Whaley, 1974; Morgenstern et al. 1975; Seinfeld,

1975; Shum et al., 1975; Ermak, 1977; Peterson and Seinfeld, 1977; Dobbins, 1979; Fisher and Macqueen, 1981; Novotny and Chesters, 1981; Wark and Warner, 1981; Karamchandani and Peters, 1983). In particular, the solution of steady state three dimensional diffusion equation with constant diffusivities and wind velocity has been obtained by incorporating settling velocity, dry deposition on the ground (Ermak, 1977). Fisher and Macqueen (1981) have solved cross wind integrated atmospheric diffusion equation under the inversion condition.

In the last few decades, the increased number of studies have been carried out to understand the scavenging of contaminant by rain (Postma, 1970; Hales, 1972, 1978, 1982a, 1982b; Slinn, 1974; Chu and Seinfeld, 1975; Scriven and Fisher, 1975a, 1975b; Peters, 1976; Maul, 1978; Barrie, 1978; Fisher, 1982; Kumar, 1985, 1986). In particular, Postma (1970) and Hales (1972) have presented some fundamentals of the precipitation scavenging of gases by rain. Hales (1972) has also called attention to the possibility that a gas plume could become redistributed in the atmosphere under the action of reversible washout. Slinn (1974) has analytically considered the redistribution of gas plume caused by reversible washout. Scriven and Fisher (1975a, 1975b) have discussed the long range transport of air borne material and its removal by deposition and washout. An excellent review of the removal processes and models of long range transport of air pollutant has been presented by Fisher (1983). A theoretical

analysis of contribution to rainwater sulfate concentration by precipitation scavenging of gaseous So_2 and sulfate (So_4^{2-}) aerosols has been presented by Peters (1976). An Eulerian model for simulating the coupled processes of gas phase depletion and aqueous phase accumulation of pollutant species has been investigated by Kumar (1985). Kumar (1986) has also extended the above Eulerian model for rain scavenging of pollutants by taking into account the process of absorption of multiple pollutant species and chemical reaction within the rain drops. The combined effects of dry deposition on the ground and various removal mechanisms such as rainout/washout, chemical reaction etc. on the dispersion of pollutants by considering them as first order process have also been studied by many workers (Astarita et al.,1979; Alam and Seinfeld, 1981). In particular, Alam and Seinfeld (1981) have discussed the dispersion of sulfur dioxide and sulfate from continuous point source and obtained analytical solution of steady state three dimensional diffusion equation by considering their removal due to rainout/washout process and dry deposition on the ground.

Peters and Richards (1977) have developed a procedure to study the steady state dispersion of pollutants from a point source with simultaneous reversible reaction when the ground surface acts as a reflecting plane. The validity of the procedure necessitates the chemical reaction to be rapid enough relative to the transport so that local chemical equilibrium is achieved at the receptor site. Shukla et al.,(1982) have

discussed the first order reverisible absorption of a pollutant from an area source in the presence of fog layer.

The dispersion of air pollutant from line source has also been studied (Walters, 1969, Dilley and Yen, 1971; Liu and Seinfeld, 1975, Sharma and Myrup, 1975, Chock, 1978, 1982; Hassid, 1983). In particular, Walter (1969) has studied the dispersion by considering uniform air velocity and taking eddy diffusivities as a linear function of height. Chock (1978) has proposed a simple linear source model to describe the downwind dispersion of pollutants near the roadways.

It is noted here that the sources of pollutant could be time dependent (for example, explosion of nuclear device such as reactor accident at Chernobyl, U.S.S.R., leakage of toxic gases from a plant as happened at Bhopal, India) and little attention has been paid to find exact solution of atmospheric diffusion equation in such cases particularly with removal mechanisms such as chemical reaction and deposition on the ground (Cleary et al. 1974; Llewelyn, 1983).

In view of this, in chapters II to V, the dispersion of reactive air pollutant from time dependent source by incorporating first order chemical kinetics and forming secondary pollutant has been discussed. In these chapters, wind velocity and diffusivities are taken as constant.

In general, the wind velocity and diffusivities are functions of space coordinates and time. In the case when

horizontal homogenity is assumed, the wind velocity and diffusion coefficients may be taken as functions of height only. For general functional forms of these variables no exact solution of three dimensional diffusion equation with chemical kinetics and other removal mechanisms is known. In few cases, however, when the wind velocity and diffusion coefficients are functions of height only, the analytical solution of steady state two dimensional diffusion equation for non reactive air pollutant has been obtained when the ground surface acts as a reflecting plane (Smith, 1957; Demuth, 1978; Robson, 1983). Heines and Peters (1974) have presented the solution of atmospheric diffusion equation (when wind speed is constant and diffusivities are function of downwind distance) by incorporating dry deposition on the ground in the model. As stated earlier, under horizontal homogenity, the meteorological variables are functions of height only. Since a general function can be approximated by a set of step functions, one way to study this kind of problems is to divide the inversion height into several layers such that the diffusion coefficients and wind velocity are assumed constants but different in different layers. The diffusion equation with these constant values is then solved in each layer with appropriate matching conditions at the interfaces of these layers. Using this concept, in Chapter VI, the steady state dispersion of reactive pollutant emitted from point and line sources is studied under inversion condition incorporating dry deposition on the ground by dividing the inversion layer into two, and three layers.

At this juncture, it may be pointed out that the pollutant in the atmosphere can be removed by introducing suitable artificial removal mechanisms to protect a given region. The mechanisms could be in the form of green belt plantation, spraying of liquid drops including water at a required place and time. It is well known that certain plants have the capability of removing pollutants in the atmosphere by absorption, deposition etc. and this property can be used for protecting a given region (Petit et al.,1976; Bache, 1979a, 1979b; Smith, 1981; Hosker et al.,1982; Slinn, 1982). In particular,the transport and deposition of particulate matters within plant and vegetable canopies have been studied. Petit et al. (1976) presented some results concerning characteristics of air flow within and above a forest by calculating So_2 fluxes at the top of the canopies. Bache (1979)ha also developed an analysis and suggested a modified form of diffusion equation to study particulate transport within and above foliage canopy. Slinn (1981) gave a theoretical frame work to predict particle deposition due to vegetation by considering wind velocity profile. A review of atmospheric deposition regarding plant assimilation of gases and particles has been presented by Smith (1981) and Hosker et al. (1982). A mathematical model for aerosol depletion and deposition on forests has also been suggested by considering a modified form of convective diffusion equation (Wiman, 1985). This model considers the interaction between forest structure and open

field by considering forest aerodynamics and aerosol characteristics.

From the above studies it may be speculated that if a suitable green belt in the form of forest is provided around the pollutant source or some distance away from it and close to the place (habitat, historical monuments, etc.) to be protected, then it is possible to reduce the concentration of pollutant by this green belt and thus protecting the region under consideration. In this direction Kapoor and Gupta (1984) studied the attenuation of an inert gas by green belt under the steady state condition.

Keeping in view of the above, the steady and unsteady state dispersion of a reactive air pollutant in the presence of green belt is studied in Chapter VII and VIII.

The removal mechanisms due to absorption of air pollutant by fog or rain droplets present in the atmosphere are very complex. In Chapter IX, a modified form of atmospheric diffusion equation is suggested in the form of an integro-partial differential equation. The effect of instantaneous and delayed removal mechanisms on the dispersion of air pollutant from an elevated time dependent point source is investigated.

1.3 SUMMARY

This thesis consists of nine chapters and deals with the steady and unsteady state dispersion of air pollutants from time

dependent sources, forming secondary pollutants, undergoing various removal mechanisms such as rainout/washout, dry deposition etc.

In Chapter I, an outline of relevant literature is presented so that the research work done in the thesis can be seen in its proper perspective.

In Chapter II, the unsteady state dispersion of a pollutant from a time dependant elevated point source undergoing first order irreversible chemical reaction and forming a secondary pollutant is discussed by assuming that these pollutants are removed by various removal processes such as rainout/washout, etc. The following forms of time dependent sources are considered : (i) instantaneous emission (ii) constant emission (iii) step function type emission.

In the case of instantaneous emission, it is shown that the concentration of both the species (primary and secondary) decreases as time increases at a particular location and the point of maximum in the concentration distance profiles moves away from the source as time passes. However, in the case of constant emission, the concentrations of both the species increase as time increases and tend to their steady state values. In the case of step function type emission (i.e. emission of pollutant occurs only upto time t_o), it is noted that for $t \leq t_o$ the concentrations of both the species increase and for $t > t_o$ the concentrations decrease as time increases.

By using the method of images, solutions are also obtained when the ground is acting as a reflecting plane. It is noted here that the solution thus obtained generalises the Gaussian puff and plume models for reactive pollutant in an isotropic atmosphere.

In Chapter III, the unsteady state dispersion of air pollutant emitted from an elevated time dependent point source undergoing first order reversible and irreversible reactions and forming a secondary pollutant is studied. It has been shown that the concentration of the primary pollutant is greater than the secondary pollutant when the forward reaction rate is less than the backward reaction rate. However, the reverse is the case when forward reaction rate is greater than the backward reaction rate. When the forward reaction rate is equal to backward reaction rate, the concentrations of both the species tend to their equilibrium values which are equal.

In Chapter IV, the unsteady state dispersion of air pollutant from a time dependent point source located at height h_s above the ground and forming a secondary pollutant is investigated by taking into account the effect of settling velocity, dry and wet depositions (without inversion condition). The analytical solution of three dimensional diffusion equation is obtained by considering wet deposition as the first order process. It is shown that as the settling velocity increases, the concentration at a point located below the source height

increases but it decreases if the point is located above the source height. It is also noted that the effect of removal process is to decrease the concentration of both primary and secondary species.

In Chapter V, the same problem is studied under the inversion condition. The comparison has been made between the two cases (with and without inversion) and it is found that the concentration of pollutant at a point with inversion condition is greater than its corresponding value in the case of without inversion condition. A particular case of the analysis presented in this chapter is applied to MIC leakage from Union Carbide Factory in Bhopal, India. This analysis provides useful information regarding impact assessment of the dispersion of MIC in Bhopal.

In previous chapters, it has been assumed that the wind speed and diffusivities are constant in the all directionsbut, in general, the wind velocity and diffusivities are functions of space coordinates and time. In the case when horizontal homogenity is assumed, the wind velocity and diffusion coefficients may be taken as functionsof height only. Since a general function can be approximated by a set of step functions, one way to study such problems is to divide the inversion height into several layers such that the wind velocity and diffusion coefficients are assumed constants but different in each layers.The diffusion equation with these constant values is then

solved in each layer with appropriate matching conditions at interfaces of these layers. Using this concept, in Chapter VI, the steady state dispersion of reactive pollutant emitted from point and line sources is studied under inversion condition by taking into account the dry deposition on the ground, dividing the inversion height into two, and three layers. The effect of stepwise variation of the wind velocity (by taking diffusion coefficients same in each layer) is to decrease the concentration of pollutant near the ground as number of layers increases. The effect of stepwise variation of the diffusion coefficients(by taking wind velocity same in each layer) is to increase the concentration of pollutant near the ground as number of layers increases.

In Chapter VII, the steady state dispersion of air pollutant from a source in the presence of green belt is studied. It is observed that the effect of green belt is to reduce the concentration of pollutant but the reduction is more if the source height is less than the average height of green belt.

In Chapter VIII, the unsteady state dispersion of reactive air pollutant in the presence of green belt is investigated. Here the whole region in the wind direction is divided into two regions, the green belt being in second region lying away from the source. It is shown that the concentration of pollutant decreases due to the presence of green belt.

In Chapter IX, a general mathematical model for atmospheric dispersion, in the form of an integro-partial differential equation is suggested where the integral term represents the removal mechanism due to absorption of air pollutant in fog/rain droplets present in the atmosphere. This model is applied to study the effects of instantaneous and delayed removal mechanisms on the dispersion of air pollutant from an elevated time dependent point source. It is shown that the concentration of the pollutant along the central line decreases due to the removal process and its magnitude in the case of delayed removal mechanism may be greater than the case of an instantaneous removal mechanism.

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CHAPTER II

UNSTEADY STATE DISPERSION OF AIR POLLUTANT FROM AN ELEVATED TIME DEPENDENT POINT SOURCE FORMING SECONDARY POLLUTANT

2.1 INTRODUCTION

The dispersion of air pollutant from a point source has been investigated by many workers using Gaussian plume and other models under various conditions (Smith, 1957; Lamb and Seinfeld, 1973;Heines and Peters 1973a, 1973b; Dobbins, 1979; Karamchandani and Peters, 1983; Llewelyn, 1983). In general, dispersal process is affected by meteorological conditions in the environment and various removal process such as chemical reaction, depositions,rainout/washout, etc. (Slinn, 1974; Seinfeld, 1975; Novotny and Chesters, 1981). For example, during dispersion SO_2 is converted to sulfate (SO_4^{2-}) aerosol in the atmosphere and both SO_2 and SO_4^{2-} are removed by wet and dry depositions. Effects of these removal mechanisms on dispersal of air pollutants have been studied by considering them as first order processes (Scriven and Fisher, 1975; Nordlund 1975; Sander and Seinfeld, 1976; McMohan et al., 1976; Prahm et al., 1976; Sheih, 1977; Calvert et al., 1978; Slinn, 1980; Alam and Seinfeld, 1981; Hale, 1982; Llewelyn,1983).

In particular, Alam and Seinfeld (1981) have studied the steady state dispersion of sulfur dioxide from a continuous point source, forming sulfate as a secondary pollutant by taking into account removal mechanisms such as deposition. In general, however, the sources of pollutant are time dependent and this aspect must be considered in the dispersal process. In such a case unsteady state diffusion equation with chemical reaction must be solved under suitable initial and boundary conditions depending upon the nature of the source (point source, line source, and area source).

Therefore, in this chapter, the dispersion of a pollutant from a time dependent elevated point source undergoing first order chemical reaction and forming a secondary pollutant has been investigated by assuming that these pollutants are removed by various processes such as rainout/washout etc. The following forms of flux at the point source have been considered in the subsequent analysis :

(1) source with instantaneous flux

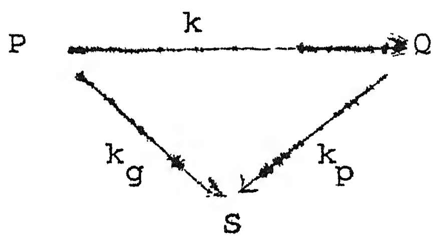
(2) source with constant flux

(3) source with step function type flux.

By using method of images, the solutions have also been obtained when the source is located at $(0,0,h_s)$ and ground is acting as a reflecting plane.

2.2 MATHEMATICAL FORMULATION

Consider the dispersion of a reactive air pollutant P, from a time dependent elevated point source in the environment undergoing first order chemical reaction and forming a secondary pollutant Q both of which are removed by mechanisms such as rainout/washout, etc. It is assumed that conversion of P into Q and their removal are first order processes with rate constants k, k_g and k_p as shown in the following scheme,



where S denotes the removal of both species from the atmosphere.

Taking the point source as the origin of the coordinate system (x,y,z), where x is in the direction of wind, the concentration of gaseous pollutant P is governed by the following atmospheric diffusion equation,

$$\frac{\partial C}{\partial t} + U\frac{\partial C}{\partial x} = D\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2}\right) - (k + k_g)\, C \tag{2.1}$$

where U is mean wind velocity assumed to be constant, D is the constant diffusion coefficient and t is the time.

The initial and boundary conditions for (2.1) can be prescribed as

$$C(s,t) = 0\ ,\ t = 0 \quad \text{for all } s = \sqrt{x^2+y^2+z^2} > 0 \tag{2.2}$$

$$C(s,t) = 0 \qquad \text{as } s \to \infty \qquad t \geq 0 \tag{2.3}$$

$$-4\pi \; s^2 D \frac{\partial C}{\partial s} = W(t) \qquad \text{as } s \to 0 \qquad t \geq 0. \tag{2.4}$$

The last boundary condition implies that the point source has time dependent flux W(t) which is considered to be of the following forms

$$\begin{aligned} &(1) \quad W(t) = W_o \; \delta(t) \\ &(2) \quad W(t) = W_c \; \text{(constant)} \\ &(3) \quad W(t) = W_c \qquad 0 \leq t \leq t_o \\ &\qquad\qquad\quad = 0 \qquad\quad t > t_o \end{aligned} \tag{2.5}$$

where $\delta(\cdot)$ is Dirac-delta function and W_o is a constant.

Similarly, the equation for the concentration C_p of the secondary species Q can be written in a coupled form (by noting the material balance of the species), as

$$\frac{\partial C_p}{\partial t} + U \frac{\partial C_p}{\partial x} = D\left(\frac{\partial^2 C_p}{\partial x^2} + \frac{\partial^2 C_p}{\partial y^2} + \frac{\partial^2 C_p}{\partial z^2}\right) + kC - k_p \; C_p \tag{2.6}$$

If there is no direct emission of the secondary pollutant then the boundary conditions for equation (2.6) can be prescribed as

$$C_p(s,t) = 0 \qquad \text{at } t = 0 \tag{2.7}$$

$$C_p(s,t) = 0 \qquad \text{as } s \to \infty, \; t \geq 0 \tag{2.8}$$

$$- 4\pi s^2 D \frac{\partial C_p}{\partial s} = 0 \quad \text{as } s \to 0, \; t \geq 0 \tag{2.9}$$

2.3 METHOD OF SOLUTION

Following Astarita et al. (1979) and Alam and Seinfeld (1981), equations (2.1) and (2.6) can be written in the compact form as

$$L \begin{bmatrix} C \\ C_p \end{bmatrix} - \begin{bmatrix} k+k_g & 0 \\ -k & k_p \end{bmatrix} \begin{bmatrix} C \\ C_p \end{bmatrix} = 0 \qquad (2.10)$$

where $L = -\frac{\partial}{\partial t} - U\frac{\partial}{\partial x} + D(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2})$ is an operator.

To uncouple this system, let us define a matrix

$$A' = \begin{bmatrix} k+k_g & 0 \\ -k & k_p \end{bmatrix} \qquad (2.11)$$

which can be written as $A' = RMR^{-1}$, where

$$R = \begin{bmatrix} 1 & 0 \\ \frac{k}{k_p-k-k_g} & 1 \end{bmatrix}, \quad M = \begin{bmatrix} k+k_g & 0 \\ 0 & k_p \end{bmatrix}, \quad R^{-1} = \begin{bmatrix} 1 & 0 \\ \frac{-k}{k_p-k-k_g} & 1 \end{bmatrix}$$

If we define a new concentration B such that

$$\begin{bmatrix} C \\ B \end{bmatrix} = R^{-1} \begin{bmatrix} C \\ C_p \end{bmatrix}, \qquad (2.12)$$

the equation (2.10) can be written in uncoupled form as

$$LC - (k+k_g)\, C = 0 \qquad (2.13)$$

$$LB - k_p\, B = 0 \qquad (2.14)$$

and from equation (2.12) we get the following relations

$$B = C_p - \frac{k\, C}{k_p-k-k_g} \qquad (2.15)$$

to find C_p once B and C are determined.

Keeping in view equations (2.2) - (2.4) and (2.7)-(2.9), the boundary conditions to determine B can then be written a

$$B(s,t) = 0 \text{ at } t = 0 \qquad (2.16)$$

$$B(s,t) = 0 \qquad \text{as } s \to \infty \text{ , } t \geq 0 \tag{2.17}$$

$$-4\pi s^2 D \frac{\partial B}{\partial s} = \frac{-k}{k_p - k - k_g} W(t) \text{ as } s \to 0, \; t \geq 0 . \tag{2.18}$$

To obtain the solution of (2.13) and (2.14) subjected to initial and boundary conditions we proceed as follows. Taking Laplace transform of equation (2.13) with respect to t and using initial condition (2.2), we have

$$U \frac{\partial \bar{C}}{\partial x} = D\left(\frac{\partial^2 \bar{C}}{\partial x^2} + \frac{\partial^2 \bar{C}}{\partial Y^2} + \frac{\partial^2 \bar{C}}{\partial z^2}\right) - m\bar{C} \tag{2.19}$$

where $\bar{C}$ is Laplace transform of C, $m = p+k+k_g$ and p is Laplace variable.

The boundary conditions become

$$\bar{C}(s,p) = 0 \qquad \text{as } s \to \infty \tag{2.20}$$

$$-4\pi s^2 D \frac{\partial \bar{C}}{\partial s} = W(p) \text{ as } s \to 0 \tag{2.21}$$

where W(p) is Laplace transform of W(t).

Assuming the solution of equation (2.19) to be of the form

$$\bar{C} = \exp\left(\frac{Ux}{2D}\right) f(s,p)$$

and using equations (2.20 - 2.21) we get

$$\bar{C} = \frac{W(p)}{4\pi D s} \exp\left[\frac{Ux}{2D} - \left(\frac{U^2}{4D^2} + \frac{m}{D}\right)^{1/2} s\right] . \tag{2.22}$$

Taking inverse Laplace transform of equation (2.22), the solution of equation (2.13) satisfying the initial and boundary conditions can be written as :

$$C(x,y,z,t) = \frac{1}{4\pi Ds}\frac{1}{2\pi i}\int_{\gamma-i\infty}^{\gamma+i\infty} W(p)\exp\left[pt+\frac{Ux}{2D}-\left(\frac{U^2}{4D^2}+\frac{m}{D}\right)^{\frac{1}{2}} s\right]dp \tag{2.23}$$

where γ is a real positive number such that all the singularities of the integrand lie on the left hand side of the line $Re(p) = \gamma$ in Bromwich contour, see fig. (2.1). Similarly, the solution of (2.14), satisfying initial and boundary conditions (2.16 - 2.17) can be written as

$$B(x,y,z,t) = \frac{A}{4\pi Ds}\frac{1}{2\pi i}\int_{\gamma-i\infty}^{\gamma+i\infty} W(p)\exp\left[pt+\frac{Ux}{2D}-\left(\frac{U^2}{4D^2}+\frac{m_1}{D}\right)^{\frac{1}{2}} s\right]dp \tag{2.24}$$

where $A = \frac{-k}{k_p-k-k_g}$, $m_1 = p + k_p$

Using Bromwich contour, the above integrals can be evaluated and we get the following expressions for concentration distributions of both the species for various forms of $W(t)$:

(i) Instantaneous flux i.e. $W(t) = W_o\,\delta(t)$

$$C(x,y,z,t) = \frac{W_o}{(4\pi Dt)^{3/2}}\exp\left[\frac{Ux}{2D}-\left(\frac{U^2}{4D}+k+k_g\right)t-\frac{s^2}{4Dt}\right] \tag{2.25}$$

$$B(x,y,z,t) = \frac{AW_o}{(4\pi Dt)^{3/2}}\exp\left[\frac{Ux}{2D}-\left(\frac{U^2}{4D}+k_p\right)t-\frac{s^2}{4Dt}\right] \tag{2.26}$$

(2) Constant flux $W(t) = W_c$

$$C(x,y,z,t) = \frac{W_c \exp(\frac{Ux}{2D})}{4\pi Ds} \{\exp\left[-(\frac{b}{D})^{1/2} s\right]$$

$$- \frac{1}{\pi} \int_b^{\infty} \frac{1}{u} e^{-ut} \sin(\frac{u-b}{D})^{1/2} s \, du\} \qquad (2.27)$$

$$B(x,y,z,t) = \frac{A \; W_c \exp(\frac{Ux}{2D})}{4\pi Ds} \{\exp\left[-(\frac{b_1}{D})^{1/2} s\right]$$

$$- \frac{1}{\pi} \int_{b_1}^{\infty} \frac{1}{u} e^{-ut} \sin(\frac{u-b_1}{D})^{1/2} s \, du\} \qquad (2.28)$$

where $b = \frac{U^2}{4D} + k + k_g$, $b_1 = \frac{U^2}{4D} + k_p$.

It is noted that expressions (2.27) and (2.28) for C and B can be obtained by integrating with respect to t the corresponding distributions given by equations (2.25) - (2.26) between 0 and t, with $W_o = W_c$.

(3) Flux as step type function i.e. $W(t) = W_c \quad 0 \le t \le t_o$

$= 0 \quad t > 0$

$$C(x,y,z,t) = \frac{W_c \exp(\frac{Ux}{2D})}{4\pi Ds} \{e^{-(\frac{b}{D})^{1/2} s} \left[1-H(t-t_o)\right]$$

$$- \frac{1}{\pi} \int_b^{\infty} \frac{1}{u} e^{-ut} \sin(\frac{u-b}{D})^{1/2} s \left[1-e^{ut_o} H(t-t_o)\right] du\}$$

(2.29)

$$B(x,y,z,t) = \frac{A \; W_c \exp(\frac{Ux}{2D})}{4\pi Ds} \{e^{-(\frac{b_1}{D})^{1/2} s} \left[1-H(t-t_o)\right]$$

$$- \frac{1}{\pi} \int_{b_1}^{\infty} \frac{1}{u} e^{-ut} \sin(\frac{u-b_1}{D})^{1/2} s \left[1-e^{ut_o} H(t-t_o)\right] du\}$$

(2.30)

where $H(t-t_o)$ is Heaviside function defined by Carslaw and Jaeger (1941) as

$$
\begin{aligned}
H(t-t_o) &= 0 \qquad t \leq t_o \\
&= \frac{t}{t_o+\varepsilon} \qquad t_o < t \leq t_o+\varepsilon \qquad (2.31)\\
&= 1 \qquad t > t_o+\varepsilon
\end{aligned}
$$

where ε can be made as small as we please.

The concentration $C_p(x,y,z,t)$ is obtained from $C(x,y,z,t)$ and $B(x,y,z,t)$ for each of the above cases using following relation

$$C_p(x,y,z,t) = B(x,y,z,t) + \frac{k\ C(x,y,z,t)}{k_p - k - k_g} \qquad (2.32)$$

where B and C are given by equations (2.25 - 2.30).

To obtain the corresponding solutions when the source is located at $(0,0,h_s)$ above a reflecting plane surface (at z=0) such that $\frac{\partial C}{\partial z} = 0$ at $z = 0$, we use the method of images for superposition of solutions as diffusion equation is linear, (Carslaw and Jaeger 1959, Dobbins, 1979 Chapter, 9). The solution of various cases are, thus, given as follows :

(1) Instantaneous flux

$$C_{11}(x,y,z,t) = \frac{W_o}{(4\pi Dt)^{3/2}} \exp\left[\frac{Ux}{2D} - bt - \left(\frac{x^2+y^2}{4Dt}\right)\right] \left\{ e^{-\frac{(z-h_s)^2}{4Dt}} + e^{-\frac{(z+h_s)^2}{4Dt}} \right\} \qquad (2.33)$$

$$B_{11}(x,y,z,t) = \frac{AW_o}{(4\pi Dt)^{3/2}} \exp\left[\frac{Ux}{2D} - b_1 \; t - \left(\frac{x^2+y^2}{4Dt}\right)\right] \{e^{-\frac{(z-h_s)^2}{4Dt}} + e^{-\frac{(z+h_s)^2}{4Dt}}\} \qquad (2.34)$$

(2) Constant flux

$$C_{21}(x,y,z,t) = \frac{W_c \exp(\frac{Ux}{2D})}{4\pi Ds_1} \{e^{-(\frac{b}{D})^{1/2} s_1} - \frac{1}{\pi}\int_b^\infty \frac{1}{u} e^{-ut} \sin(\frac{u-b}{D})^{1/2} s_1 du\}$$

$$+ \frac{W_c \exp(\frac{Ux}{2D})}{4\pi Ds_2} \{e^{-(\frac{b}{D})^{1/2} s_2} - \frac{1}{\pi}\int_b^\infty \frac{1}{u} e^{-ut} \sin(\frac{u-b}{D})^{1/2} s_2 du\} \qquad (2.35)$$

$$B_{21}(x,y,z,t) = \frac{AW_c \exp(\frac{Ux}{2D})}{4\pi Ds_1} \{e^{-(\frac{b_1}{D})^{1/2} s_1}$$

$$- \frac{1}{\pi}\int_{b_1}^\infty \frac{1}{u} e^{-ut} \sin(\frac{u-b_1}{D})^{1/2} s_1 du\}$$

$$+ \frac{AW_c \exp(\frac{Ux}{2D})}{4\pi Ds_2} \{e^{-(\frac{b_1}{D})^{1/2} s_2}$$

$$- \frac{1}{\pi}\int_{b_1}^\infty \frac{1}{u} e^{-ut} \sin(\frac{u-b_1}{D})^{1/2} s_2 du\} \qquad (2.36)$$

(3) Step function type flux

$$C_{31}(x,y,z,t) = \frac{W_c \exp(\frac{Ux}{2D})}{4\pi Ds_1} \{e^{-(\frac{b}{D})^{1/2} s_1} [1-H(t-t_o)]$$

$$- \frac{1}{\pi}\int_b^\infty \frac{1}{u} e^{-ut} \sin(\frac{u-b}{D})^{1/2} s_1 [1-e^{ut_o} H(t-t_o)] du\}$$

$$+ \frac{W_c \exp(\frac{Ux}{2D})}{4\pi Ds_2} \{e^{-(\frac{b}{D})^{1/2} s_2} [1-H(t-t_o)]$$

$$- \frac{1}{\pi} \int_{b}^{\infty} \frac{1}{u} e^{-ut} \sin \left(\frac{u-b}{D}\right)^{1/2} s_2 \left[1-e^{ut_o} H(t-t_o)\right] du\} \quad (2.37)$$

$$B_{31}(x,y,z,t) = \frac{A\ W_c(\exp(\frac{Ux}{2D})}{4\pi D s_1} \{ e^{-(\frac{b_1}{D})^{1/2} s_1} \left[1-H(t-t_o)\right]$$

$$- \frac{1}{\pi} \int_{b_1}^{\infty} \frac{1}{u} e^{-ut} \sin\left(\frac{u-b_1}{D}\right)^{1/2} s_1 \left[1-e^{ut_o} H(t-t_o)\right] du\}$$

$$+ \frac{A\ W_c \exp(\frac{Ux}{2D})}{4\pi D s_2} \{ e^{-(\frac{b_1}{D})^{1/2} s_2} \left[1-H(t-t_o)\right]$$

$$- \frac{1}{\pi} \int_{b_1}^{\infty} \frac{1}{u} e^{-ut} \sin\left(\frac{u-b_1}{D}\right)^{1/2} s_2 \left[1-e^{ut_o} H(t-t_o)\right] du\} \quad (2.38)$$

where $s_1^2 = x^2+y^2+(z-h_s)^2$, $s_2^2 = x^2+y^2+(z+h_s)^2$.

It is found that equations (2.37) and (2.38) can also be obtained by following relations

$$C_{31}(x,y,z,t) = \int_0^t C_{11}(x,y,z,t')dt' - H(t-t_o) \int_0^{t-t_o} C_{11}(x,y,z,t')dt' \quad (2.39)$$

$$B_{31}(x,y,z,t) = \int_0^t B_{11}(x,y,z,t')dt' - H(t-t_o) \int_0^{t-t_o} B_{11}(x,y,z,t')\ dt' \quad (2.40)$$

and $W_o = W_c$.

Here the concentration C_p can be obtained from equation (2.15) by substituting C_{i1} and B_{i1} ($i = 1,2,3$) in place of C and B respectively.

For the steady state constant flux case, equations (2.35 - 2.36) reduce to following forms

$$C_{21}(x,y,z,t) = \frac{W_c \exp(\frac{Ux}{2D})}{4\pi D}\left[\frac{e^{-(\frac{b}{D})^{1/2} s_1}}{s_1} + \frac{e^{-(\frac{b}{D})^{1/2} s_2}}{s_2}\right] \quad (2.41)$$

$$B_{21}(x,y,z,t) = \frac{AW_c \exp(\frac{Ux}{2D})}{4\pi D}\left[\frac{e^{-(\frac{b_1}{D})^{1/2} s_1}}{s_1} + \frac{e^{-(\frac{b_1}{D})^{1/2} s_2}}{s_2}\right] \quad (2.42)$$

Taking $\frac{y^2+(z-h_s)^2}{x^2} << 1$, $\frac{y^2+(z+h_s)^2}{x^2} << 1$ $\frac{(k+k_g)D}{u^2} << 1$ and $\frac{k_p D}{u^2} << 1$, then the linearized form of solution can be obtained as

$$C_{21}(x,y,z,t) = \frac{W_c}{4\pi Dx} \exp\left[-(\frac{k+k_g}{U})x - \frac{U^2y^2}{4Dx}\right] \times$$

$$\left\{\exp\left[-\frac{U(z-h_s)^2}{4Dx}\right] + \exp\left[-\frac{U(z+h_s^2)}{4Dx}\right]\right\} \quad (2.43)$$

$$B_{21}(x,y,z,t) = \frac{A\ W_c}{4\pi Dx} \exp\left[-\frac{k_p x}{U} - \frac{U^2y^2}{4Dx}\right] \times$$

$$\left\{\exp\left[-\frac{U(z-h_s)^2}{4Dx}\right] + \exp\left[-\frac{U(z+h_s)^2}{4Dx}\right]\right\} \quad (2.44)$$

To compare present model with Gaussian plume model (which is commonly used), we make further transformations according to the relation,

$$\sigma^2 = \frac{2Dx}{U}$$

and we get

$$C_{21}(x,y,z,t) = \frac{W_c}{2\pi\sigma^2 U} \exp\left[-\left(\frac{k+k_g}{U}\right)x - \frac{y^2}{2\sigma^2}\right] \times \left\{e^{-\frac{(z-h_s)^2}{2\sigma^2}} + e^{-\frac{(z+h_s)^2}{2\sigma^2}}\right\} \quad (2.45)$$

$$B_{21}(x,y,z,t) = \frac{A\ W_c}{2\pi\sigma^2 U} \exp\left[-\frac{k_p x}{U} - \frac{y^2}{2\sigma^2}\right] \times \left\{e^{\frac{-(z-h_s)^2}{2\sigma^2}} + e^{\frac{-(z+h_s)^2}{2\sigma^2}}\right\} \quad (2.46)$$

Putting $k = k_g = k_p = 0$, it is straight forward to reduce these expressions to standard form for a continuous Gaussian plume model in the isotropic media. It may be observed that the solution for Gaussian puff model to non reactive pollutant has been extended to a reactive pollutant forming secondary pollutant in an isotropic media.

2.4 RESULTS AND DISCUSSION

To see the effects of various parameters on the concentration distributions of both the species in each case, we use following dimensionless quantities:

$$\bar{t} = \frac{D}{h_s^2}t\ ,\ \bar{x} = \frac{x}{h_s}\ ,\ \bar{y} = \frac{y}{h_s}\ ,\ \bar{z} = \frac{z}{h_s}\ ,\ \bar{k} = \frac{h_s^2\ k}{D}\ ,\ \bar{k}_g = \frac{k_g\ h_s^2}{D}\ ,$$

$$\bar{k}_p = \frac{k_p\ h_s^2}{D}\ ,\ \bar{U} = \frac{U\ h_s}{D}\ ,\ \bar{C} = \frac{h_s D}{W_c}C\ ,\ \bar{C}_p = \frac{h_s D C_p}{W_c}\ ,\bar{W}_o = \frac{W_o\ D}{W_c h_s^2} \quad (2.47)$$

Equations (2.33 - 2.34) can be written in dimensionless form for each case as follows (dropping bars for convenience):

(i) Instantaneous flux

$$C_{11}(x,y,z,t) = \frac{W_o}{(4\pi t)^{3/2}} \exp\left[\frac{Ux}{2} - bt - \left(\frac{x^2+y^2}{4t}\right)\right] \times$$

$$\left\{e^{-\frac{(z-1)^2}{4t}} + e^{-\frac{(z+1)^2}{4t}}\right\} \qquad (2.48)$$

$$B_{11}(x,y,z,t) = \frac{A\ W_o}{(4\pi t)^{3/2}} \exp\left[\frac{Ux}{2} - b_1 t - \frac{(x^2+y^2)}{4t}\right] \times$$

$$\left\{e^{-\frac{(z-1)^2}{4t}} + e^{-\frac{(z+1)^2}{4t}}\right\} \qquad (2.49)$$

where b and b_1 (dimensionless form) are

$$b = \frac{U^2}{4} + k + k_g \ , \ b_1 = \frac{U^2}{4} + k_p$$

(ii) Constant flux

$$C_{21} = \int_0^t C_{11}(x,y,z,t')\ dt' \qquad (2.50)$$

$$B_{21} = \int_0^t B_{11}(x,y,z,t')\ dt' \qquad (2.51)$$

(iii) Step function type flux

$$C_{31} = \int_0^t C_{11}(x,y,z,t')dt' - H(t-t_o) \int_0^{t-t_o} C_{11}(x,y,z,t')\ dt' \qquad (2.52)$$

$$B_{31} = \int_0^t B_{11}(x,y,z,t')dt' - H(t-t_o) \int_0^{t-t_o} B_{11}(x,y,z,t')\, dt' \tag{2.53}$$

To see the effects of various parameters on the dimensionless ground level concentration, the expressions for C and C_p given by equations (2.48 - 2.53) are calculated, by choosing the following set of values of parameters :

$W_o = 1.0$, $U = 5.0$, $k = 0.11$, $k_g = 0.0, 0.08$,

$k_p = 0.0, 0.8$, $y = 0.0$ and depicted in figs.(2.2 - 2.8).

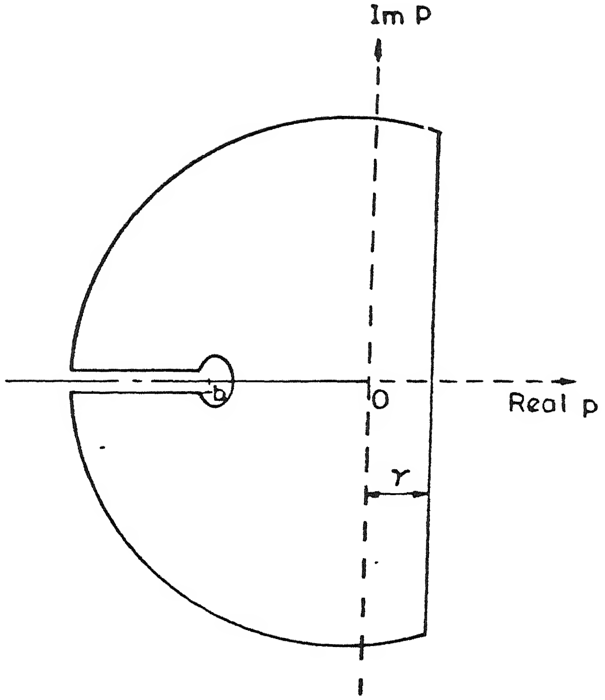
It is observed that the concentrations C, C_p decrease as downwind distance increases. It is noted that as p increases C decreases but C_p increases in all cases at a particular time and location (see fig. 2.6).

When the flux is instantaneous at the source, the dimensionless concentrations C and C_p are shown in figs.(2.2 - 2.3) for different values of t and $W_o = 1.0$. It is noted from these figures that as time increases both C and C_p decrease and the point of maxima in the concentration distance profile of each species moves away from the source.

For the case of constant flux, the ground level dimensionless concentrations C and C_p are shown in figs. (2.4 - 2.6) for different values of t. It is seen from these figs. that both C and C_p increase as time increases and would eventually tend to their steady state values.

For the case of step function type flux, the ground level concentration is plotted in figs. (2.7 - 2.8). These figs. show that concentrations C and C_p decrease as time t increases for $t > t_o$. However for $t \leq t_o$, the profiles for C and C_p are similar to the case of constant flux.

The effect of removal mechanisms on C and C_p can be seen by comparing the figs. 2.2 and 2.3, 2.4 and 2.5, 2.7 and 2.8. It is observed that C and C_p decrease as k_g and k_p increase respectively.



BROMWICH CONTOUR

FIG 2.1

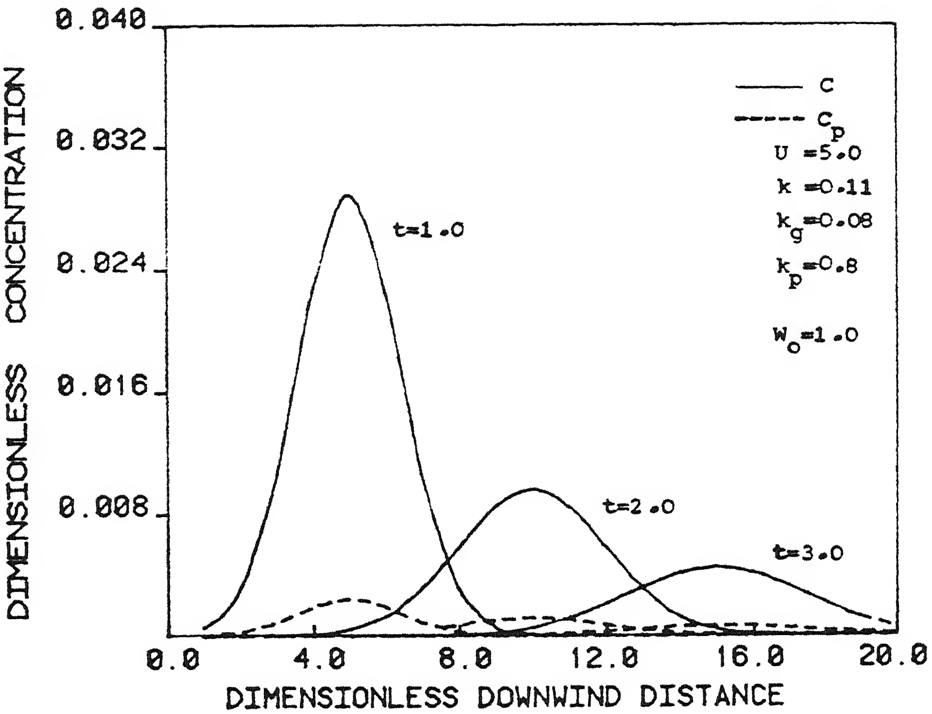


FIG 2.2 FLUX IS INSTANTANEOUS AT THE SOURCE

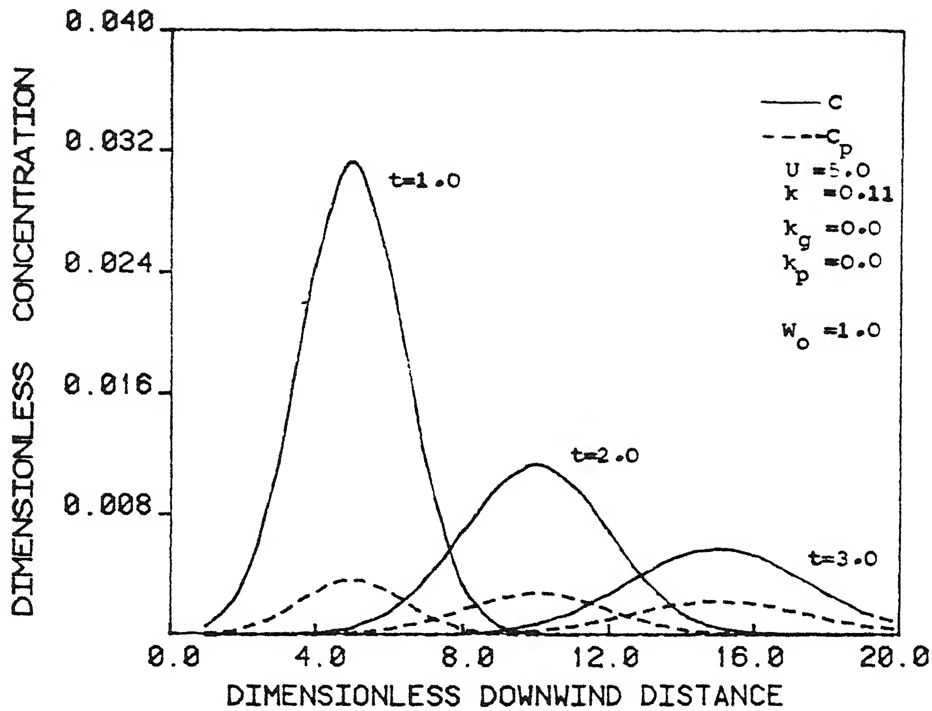


FIG 2.3 FLUX IS INSTANTANEOUS AT THE SOURCE

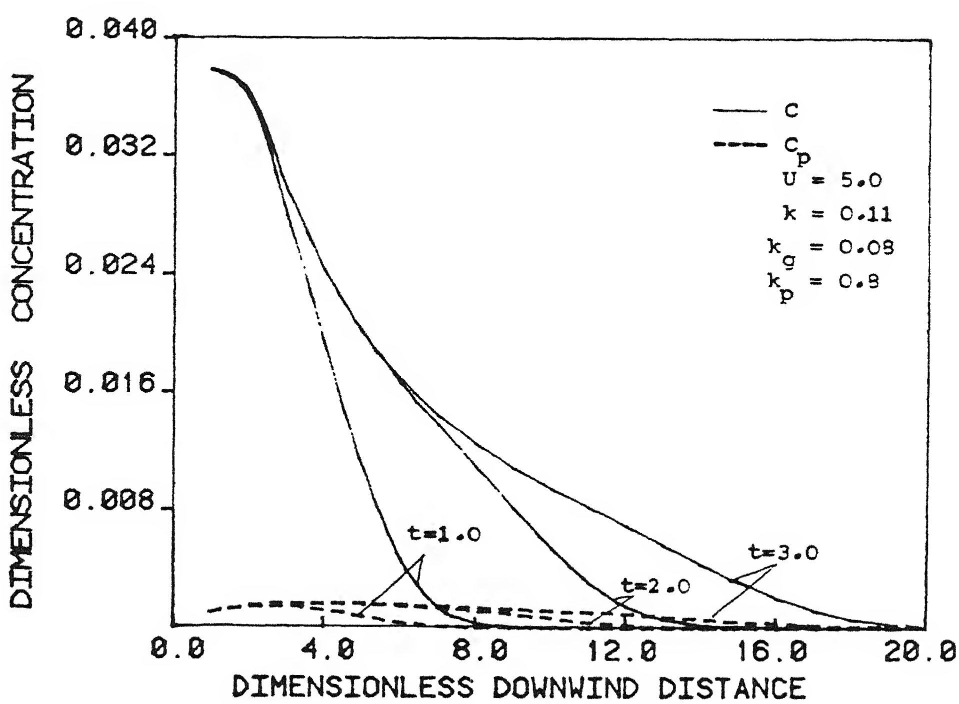


FIG2.4 FLUX IS CONSTANT AT THE SOURCE

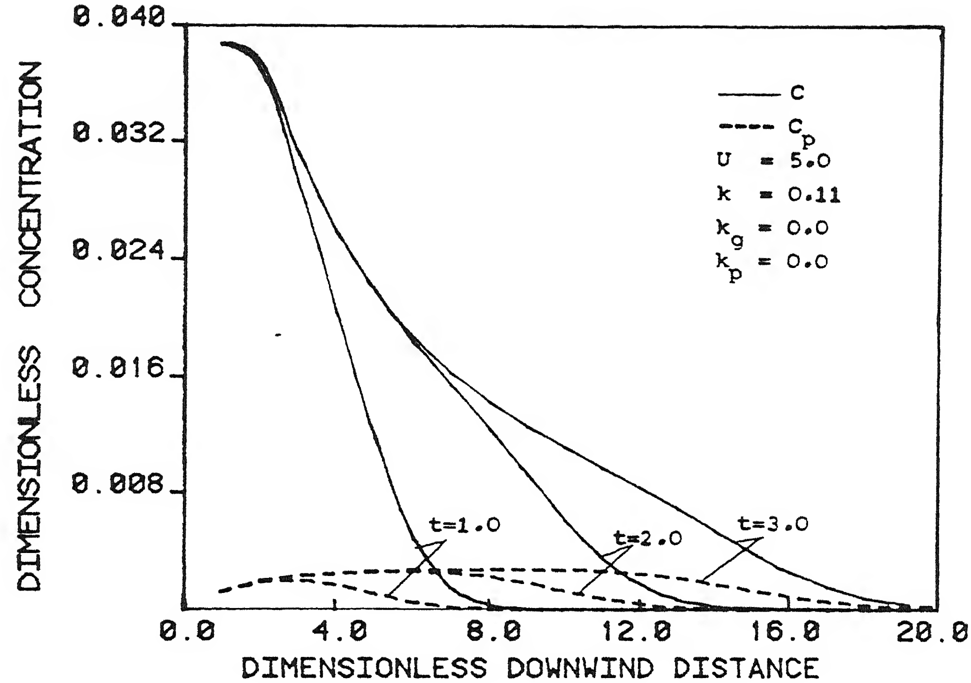


FIG2.5 FLUX IS CONSTANT AT THE SOURCE

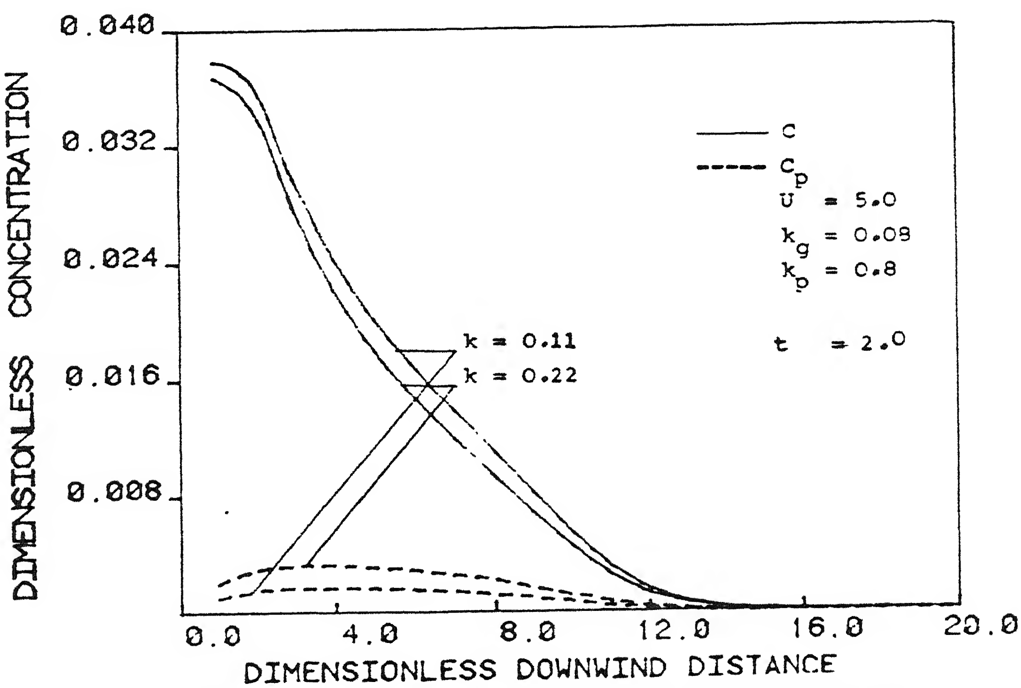


FIG.2.6 FLUX IS CONSTANT AT THE SOURCE

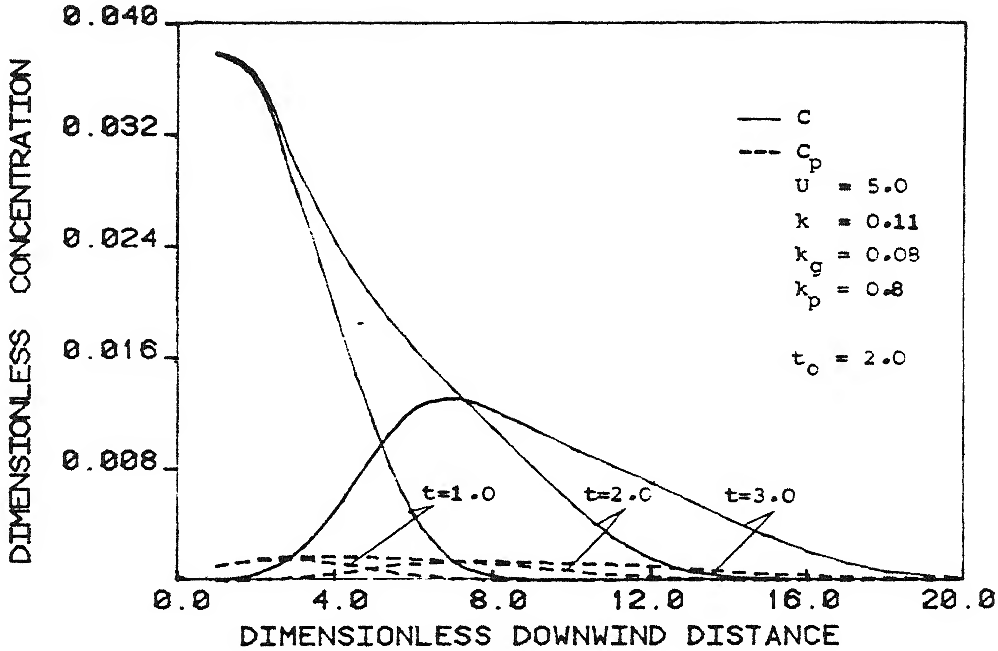


FIG 2.7 FLUX IS STEP FUNCTION TYPE AT THE SOURCE

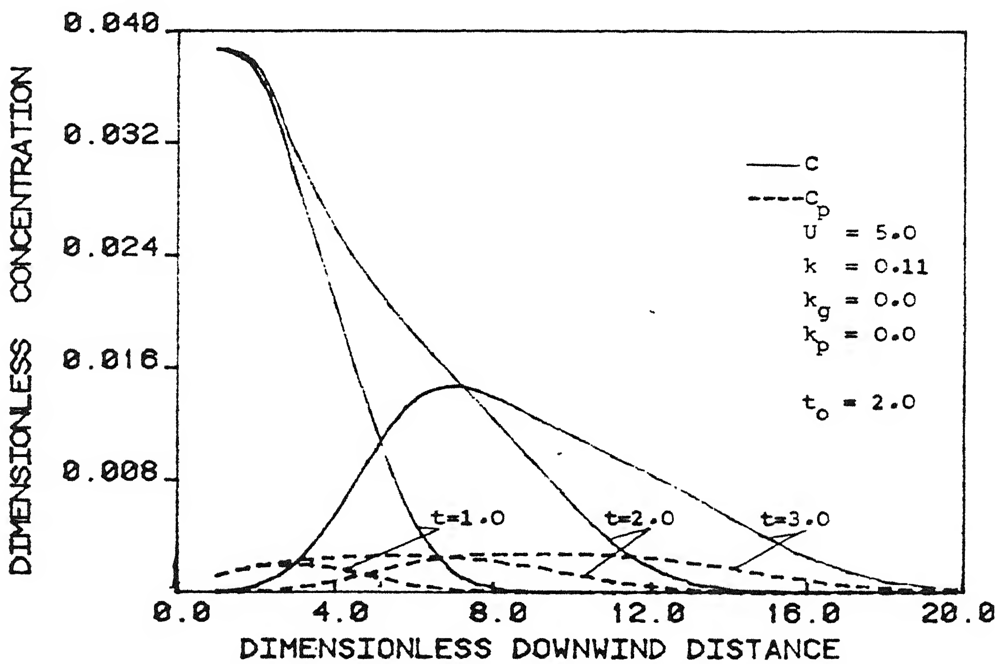


FIG2.8 FLUX IS STEP FUNCTION TYPE AT THE SOURCE

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CHAPTER III

UNSTEADY STATE DISPERSION OF AIR POLLUTANT FROM AN ELEVATED TIME DEPENDENT POINT SOURCE UNDERGOING FIRST ORDER IRREVERSIBLE AND REVERSIBLE PROCESSES

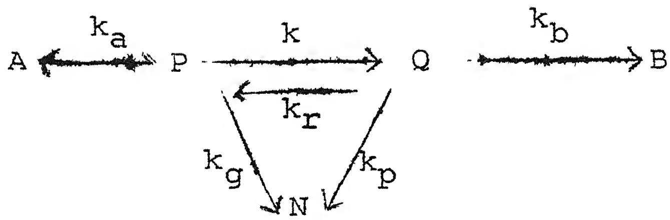
3.1 INTRODUCTION

The dispersion of air pollutant from a time dependent point source undergoing first order irreversible chemical reaction has been discussed in Chapter II. Since there are situations in the atmosphere where the formation of secondary pollutant is accompanied by a reversible reaction, this aspect must also be studied (Peters and Richards, 1977, Shukla et al., 1982).

Therefore, in this chapter, the unsteady state dispersion of a reactive air pollutant emitted from an elevated time dependent point source undergoing first order reversible and irreversible reactions forming secondary pollutant have been discussed.

3.2 MATHEMATICAL FORMULATION

Consider the dispersion of a reactive gaseous pollutant P, emitted from a time dependent elevated point source, undergoing first order reversible reaction forming secondary pollutant Q and both P and Q react irreversibily with species present in the atmosphere. The scheme of their reactions can be described as follows:



where k, k_r, k_a, k_b are rates of reversible and irreversible chemical reactions, k_g, k_p are the removal rates of P and Q due to removal mechanisms present in the atmosphere such as rainout/washout.

The concentration of gaseous pollutant P is governed by the following diffusion equation under the assumption that the eddy diffusivities are uniform in all directions (= D, say)

$$\frac{\partial C}{\partial t} + U\frac{\partial C}{\partial x} = D\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2}\right) - (k+k_a+k_g)\,C + k_r C_p \qquad (3.1)$$

where U is the wind velocity taken along the x-direction and C_p is the concentration of secondary pollutant Q.

Taking the source as origin of the coordinate system, the initial and boundary conditions are given by

$$C(s,t) = 0 \quad t = 0 \text{ for } s = \sqrt{x^2+y^2+z^2} > 0 \qquad (3.2)$$

$$C(s,t) = 0 \quad \text{as } s \to \infty \quad t \geq 0 \qquad (3.3)$$

$$-4\pi s^2 D\frac{\partial C}{\partial s} = W(t) \quad \text{as } s \to 0 \quad t \geq 0. \qquad (3.4)$$

The last boundary condition implies that the point source has time dependent flux W(t). The following forms of W(t) are considered for subsequent analysis :

(i) Instantaneous flux at the source

$W(t) = W_o \, \delta(t)$

(ii) Constant flux at the source

$$W(t) = W_c \tag{3.5}$$

(iii) Step function type flux at the source

$$W(t) = W_c \qquad 0 < t \leq t_o$$
$$= 0 \qquad t > t_o$$

Under similar assumptions the transport equation governing the concentration C_p of the secondary pollutant Q can be written as

$$\frac{\partial C_p}{\partial t} + U \frac{\partial C_p}{\partial x} = D_p \left(\frac{\partial^2 C_p}{\partial x^2} + \frac{\partial^2 C_p}{\partial y^2} + \frac{\partial^2 C_p}{\partial z^2}\right) + kC - (k_r + k_b + k_p)C_p \tag{3.6}$$

where D_p is diffusion coefficient of secondary pollutant.

The initial and boundary conditions for C_p can be written (assuming that there is no direct emission of secondary pollutant) as

$$C_p(s,t) = 0 \quad t = 0 \quad \text{for } s > 0 \tag{3.7}$$

$$C_p(s,t) = 0 \quad \text{as } s \to \infty \qquad t \geq 0 \tag{3.8}$$

$$-4\pi s^2 D_p \frac{\partial C_p}{\partial s} = 0 \text{ as } s \to 0 \quad t \geq 0 \,. \tag{3.9}$$

3.3 METHOD OF SOLUTION

Assuming that primary and secondary pollutants are dispersed in the atmosphere in same manner, in the following analysis we take $D_p = D$. In such a case, taking Laplace transform of equations (3.1) and (3.6) with respect to t, we get

$$U \frac{\partial \bar{C}}{\partial x} = D\left(\frac{\partial^2 \bar{C}}{\partial x^2} + \frac{\partial^2 \bar{C}}{\partial y^2} + \frac{\partial^2 \bar{C}}{\partial z^2}\right) - (k+k_a+k_g+p)\bar{C} + k_r \bar{C}_p \qquad (3.10)$$

$$U \frac{\partial \bar{C}_p}{\partial x} = D\left(\frac{\partial^2 \bar{C}_p}{\partial x^2} + \frac{\partial^2 \bar{C}_p}{\partial y^2} + \frac{\partial^2 \bar{C}_p}{\partial z^2}\right) - (k_b+k_r+k_p+p)\bar{C}_p + k\bar{C} \qquad (3.11)$$

where $\bar{C}$ and $\bar{C}_p$ are the Laplace transforms of C and C_p respectively, p being Laplace variable.

The boundary conditions for $\bar{C}$ and $\bar{C}_p$ become

$$\bar{C}(s,p) = 0 \quad \text{as } s \to \infty \qquad (3.12)$$

$$-4\pi s^2 D \frac{\partial \bar{C}}{\partial s} = W(p) \quad \text{as } s \to 0 \qquad (3.13)$$

$$\bar{C}_p(s,p) = 0 \quad \text{as } s \to \infty \qquad (3.14)$$

$$-4\pi s^2 D \frac{\partial \bar{C}_p}{\partial s} = 0 \text{ as } s \to 0 \qquad (3.15)$$

where W(p) is Laplace transform of W(t).

Assuming that the concentration distributions for both the species are of the following forms

$$\bar{C} = e^{\left(\frac{Ux}{2D}\right)} f_1(s,p) \qquad (3.16)$$

$$\bar{C}_p = e^{(\frac{Ux}{2D})} \; f_2(s,p) \tag{3.17}$$

the equations (3.10) and (3.11) become

$$(D'^2 - m_1) s \; f_1(s,p) + \frac{k_r}{D} \; s \; f_2(s,p) = 0 \tag{3.18}$$

$$(D'^2 - m_2) s \; f_2(s,p) + \frac{k}{D} \; s \; f_1(s,p) = 0 \tag{3.19}$$

where

$$m_1 = \frac{U^2}{4D^2} + \frac{k+k_a+k_g+p}{D} \; , \; m_2 = \frac{U^2}{4D^2} + \frac{k_r+k_b+k_p+p}{D}$$

and $D' = \frac{d}{ds}$.

Solving equations (3.18), (3.19) and using the corresponding boundary conditions, the expressions for $\bar{C}$ and $\bar{C}_p$ have been obtained as

$$\bar{C} = \frac{W(p)}{4\pi DS} \{ - \frac{(\frac{m'-n'}{2} - M)}{2M} \; e^{\frac{Ux}{2D} - (\frac{p}{D} + \frac{m'+n'}{2D} - \frac{M}{D})^{1/2} s}$$

$$+ \frac{(\frac{m'-n'}{2} + M)}{2M} \; e^{\frac{Ux}{2D} - (\frac{p}{D} + \frac{m'+n'}{2D} + \frac{M}{D})^{1/2} s} \} \tag{3.20}$$

$$\bar{C}_p = \frac{W(p)}{4\pi DS} \; \frac{k}{2M} \; [e^{\frac{Ux}{2D} - (\frac{p}{D} + \frac{m'+n'}{2D} - \frac{M}{D})^{1/2} s}$$

$$- e^{\frac{Ux}{2D} - (\frac{p}{D} + \frac{m'+n'}{2D} + \frac{M}{D})^{1/2} s}] \tag{3.21}$$

where

$$m' = \frac{U^2}{4D} + k + k_g + k_a$$

$$n' = \frac{U^2}{4D} + k_r + k_b + k_p$$

$$M = \{(\frac{m'-n'}{2})^2 + k\, k_r\}^{1/2}.$$

Taking inverse Laplace transform of expressions (3.20) - (3.21) by using Bromwich contour (Carslaw and Jaeger, 1941), the following expressions for concentration distribution for both the species are obtained in each case as follows :

(i) Instantaneous flux .

$$C(x,y,z,t) = \frac{W_o}{(4\pi Dt)^{3/2}} \{\frac{b_2}{2M} \exp\left[\frac{Ux}{2D} - b_1't - \frac{s^2}{4Dt}\right]$$

$$+ \frac{b_3}{2M} \exp\left[\frac{Ux}{2D} - b't - \frac{s^2}{4Dt}\right]\} \tag{3.22}$$

$$C_p(x,y,z,t) = \frac{W_o}{(4\pi Dt)^{3/2}} \frac{k}{2M} \{\exp\left[\frac{Ux}{2D} - b_1't - \frac{s^2}{4Dt}\right]$$

$$- \exp\left[\frac{Ux}{2D} - b't - \frac{s^2}{4Dt}\right]\} \tag{3.23}$$

(ii) Constant flux (Continuous source)

$$C(x,y,z,t) = \frac{W_c \exp(\frac{Ux}{2D})}{4\pi Ds} \left[\frac{b_2}{2M} \{e^{-(\frac{b_1'}{D})^{1/2} s}\right.$$

$$- \frac{1}{\pi} \int_{b_1'}^{\infty} \frac{1}{u} e^{-ut} \sin\left(\frac{u-b_1'}{D}\right)^{1/2} s \, du\}$$

$$\left. + \frac{b_3}{2M}\{e^{-(\frac{b'}{D})^{1/2} s} - \frac{1}{\pi} \int_{b'}^{\infty} \frac{1}{u} e^{-ut} \sin\left(\frac{u-b'}{D}\right)^{1/2} s \, du\}\right] \tag{3.24}$$

$$C_p(x,y,z,t) = \frac{W_c \exp(\frac{Ux}{2D})}{4\pi Ds} \frac{k}{2M} [e^{-(\frac{b_1'}{D})^{1/2}s}$$

$$- \frac{1}{\pi} \int_{b_1'}^{\infty} \frac{1}{u} e^{-ut} \sin(\frac{u-b_1'}{D})^{1/2} s \, du$$

$$- e^{-(\frac{b'}{D})^{1/2}s} + \frac{1}{\pi} \int_{b'}^{\infty} \frac{1}{u} e^{-ut} \sin(\frac{u-b'}{D})^{1/2} s \, du]$$

(3.25)

(iii) Step function type flux

$$C(x,y,z,t) = \frac{W_c \exp(\frac{Ux}{2D})}{4\pi Ds} [\frac{b_2}{2M} \{e^{-(\frac{b_1'}{D})^{1/2}s} (1-H(t-t_o))$$

$$- \frac{1}{\pi} \int_{b_1'}^{\infty} \frac{1}{u} e^{-ut} [1-e^{ut_o} H(t-t_o)] \sin(\frac{u-b_1'}{D})^{1/2} s \, du\}$$

$$+ \frac{b_3}{2M} \{e^{-(\frac{b'}{D})^{1/2}s} (1-H(t-t_o))$$

$$- \frac{1}{\pi} \int_{b'}^{\infty} \frac{1}{u} e^{-ut} [1-e^{ut_o} H(t-t_o)] \sin(\frac{u-b'}{D})^{1/2} s \, du\}]$$

(3.26)

$$C_p(x,y,z,t) = \frac{W_c \exp(\frac{Ux}{2D})}{4\pi Ds} \frac{k}{2M} \{e^{-(\frac{b_1'}{D})^{1/2}s} (1-H(t-t_o))$$

$$- \frac{1}{\pi} \int_{b_1'}^{\infty} \frac{1}{u} e^{-ut} [1-e^{ut_o} H(t-t_o)] \sin(\frac{u-b_1'}{D})^{1/2} s \, du$$

$$- e^{-(\frac{b'}{D})^{1/2}s} (1-H(t-t_o))$$

$$+ \frac{1}{\pi} \int_{b'}^{\infty} \frac{1}{u} e^{-ut} [1-e^{ut_o} H(t-t_o)] \sin(\frac{u-b'}{D})^{1/2} s \, du\}$$

(3.27)

where $b' = \frac{m'+n'}{2} + M$, $b_1' = \frac{m'+n'}{2} - M$

$$b_2 = -\frac{m'-n'}{2} + M, b_3 = \frac{m'-n'}{2} + M.$$

To obtain the corresponding solution when the source is located at $(0,0,h_s)$ above a reflecting plane (at $z = 0$) such that $\frac{\partial C}{\partial z} = 0$ at $z = 0$, we use the method of images for superposition of solutions since diffusion equation is linear (Dobbins, 1979; Carslaw and Jaeger, 1959).

The solution for various cases are :

(i) Instantaneous flux

$$C_1(x,y,z,t) = \frac{W_o \exp(\frac{Ux}{2D})}{(4\pi Dt)^{3/2}} \{\frac{b_2}{2M} e^{-b_1' t} [e^{-\frac{s_1^2}{4Dt}} + e^{-\frac{s_2^2}{4Dt}}]$$

$$+ \frac{b_3}{2M} e^{-b't} [e^{-\frac{s_1^2}{4Dt}} + e^{-\frac{s_2^2}{4Dt}}]\} \qquad (3.28)$$

$$C_{p1}(x,y,z,t) = \frac{W_o \exp(\frac{Ux}{2D})}{(4\pi Dt)^{3/2}} \frac{k}{2M} \{e^{-b_1' t} [e^{-\frac{s_1^2}{4Dt}} + e^{-\frac{s_2^2}{4Dt}}]$$

$$- e^{-b't}[e^{-\frac{s_1^2}{4Dt}} + e^{-\frac{s_2^2}{4Dt}}]\} \qquad (3.29)$$

(ii) Constant flux

$$C_2(x,y,z,t) = \frac{W_c \exp(\frac{Ux}{2D})}{4\pi D} [\frac{b_2}{2M} \{\frac{e^{-(\frac{b_1'}{D})^{1/2} s_1}}{s_1} + \frac{e^{-(\frac{b_1'}{D})^{1/2} s_2}}{s_2}$$

$$- \frac{1}{\pi s_1} \int_{b_1'}^{\infty} \frac{1}{u} e^{-ut} \sin(\frac{u-b_1'}{D})^{1/2} s_1 \, du$$

$$- \frac{1}{\pi s_2} \int_{b_1'}^{\infty} \frac{1}{u} e^{-ut} \sin(\frac{u-b_1'}{D})^{1/2} s_2 du\}$$

$$\frac{b_3}{2M}\{\frac{e^{-(\frac{b'}{D})^{1/2}s_1}}{s_1} + \frac{e^{-(\frac{b'}{D})^{1/2}s_2}}{s_2}$$

$$- \frac{1}{\pi s_1}\int_{b'}^{\infty} \frac{1}{u} e^{-ut} \sin(\frac{u-b'}{D})^{1/2}s_1\, du$$

$$- \frac{1}{\pi s_2}\int_{b'}^{\infty} \frac{1}{u} e^{-ut} \sin(\frac{u-b'}{D})^{1/2}s_2\, du\}] \qquad (3.30)$$

$$C_{p2}(x,y,z,t) = \frac{W_c \exp(\frac{Ux}{2D})}{4\pi D}\frac{k}{2M}[\{\frac{e^{-(\frac{b_1'}{D})^{1/2}s_1}}{s_1} + \frac{e^{-(\frac{b_1'}{D})^{1/2}s_2}}{s_2}$$

$$- \frac{1}{\pi s_1}\int_{b_1'}^{\infty} \frac{1}{u} e^{-ut} \sin(\frac{u-b_1'}{D})^{1/2}s_1\, du$$

$$- \frac{1}{\pi s_2}\int_{b_1'}^{\infty} \frac{1}{u} e^{-ut} \sin(\frac{u-b_1'}{D})^{1/2}s_2\, du\}$$

$$-\{\frac{e^{-(\frac{b'}{D})^{1/2}s_1}}{s_1} + \frac{e^{-(\frac{b'}{D})^{1/2}s_2}}{s_2}$$

$$- \frac{1}{\pi s_1}\int_{b'}^{\infty} \frac{1}{u} e^{-ut} \sin(\frac{u-b'}{D})^{1/2}s_1\, du$$

$$- \frac{1}{\pi s_2}\int_{b'}^{\infty} \frac{1}{u} e^{-ut} \sin(\frac{u-b'}{D})^{1/2}s_2\, du\}] \qquad (3.31)$$

(iii) Step function type flux

$$C_3(x,y,z,t) = \frac{W_c \exp(\frac{Ux}{2D})}{4\pi D}[\frac{b_2}{2M}\{(1-H(t-t_o))\{\frac{e^{-(\frac{b_1'}{D})^{1/2}s_1}}{s_1} + \frac{e^{-(\frac{b_1'}{D})^{\frac{1}{2}}s_2}}{s_2}\}$$

$$- \frac{1}{\pi s_1}\int_{b_1'}^{\infty} \frac{1}{u} e^{-ut} [1-e^{ut_o}H(t-t_o)] \sin(\frac{u-b_1'}{D})^{1/2}s_1\, du$$

$$- \frac{1}{\pi s_2}\int_{b_1'}^{\infty} \frac{1}{u} e^{-ut} [1-e^{ut_o}H(t-t_o)] \sin(\frac{u-b_1'}{D})^{1/2}s_2\, du\}$$

$$+ \frac{b_3}{2M} \{ (\frac{e^{-(\frac{b'}{D})^{1/2} s_1}}{s_1} + \frac{e^{-(\frac{b'}{D})^{1/2} s_2}}{s_2})(1-H(t-t_o))$$

$$- \frac{1}{\pi s_1} \int_{b'}^{\infty} \frac{1}{u} e^{-ut} [1-e^{ut_o} H(t-t_o)] \sin(\frac{u-b'}{D})^{1/2} s_1 \, du$$

$$- \frac{1}{\pi s_2} \int_{b'}^{\infty} \frac{1}{u} e^{-ut} [1-e^{ut_o} H(t-t_o)] \sin(\frac{u-b'}{D})^{1/2} s_2 \, du\}]$$

$$(3.32)$$

$$C_{p3}(x,y,z,t) = \frac{W_c \exp(\frac{Ux}{2D})}{4\pi D} \frac{k}{2M} \{ (\frac{e^{-(\frac{b'_1}{D})^{1/2} s_1}}{s_1} + \frac{e^{-(\frac{b'_1}{D})^{\frac{1}{2}} s_2}}{s_2})(1-H(t-t_o))$$

$$- \frac{1}{\pi s_1} \int_{b'_1}^{\infty} \frac{1}{u} e^{-ut} [1-e^{ut_o} H(t-t_o)] \sin(\frac{u-b'_1}{D})^{1/2} s_1 \, du$$

$$- \frac{1}{\pi s_2} \int_{b'_1}^{\infty} \frac{1}{u} e^{-ut} [1-e^{ut_o} H(t-t_o)] \sin(\frac{u-b'_1}{D})^{1/2} s_2 \, du$$

$$- (\frac{e^{-(\frac{b'}{D})^{1/2} s_1}}{s_1} + \frac{e^{-(\frac{b'}{D})^{1/2} s_2}}{s_2})(1-H(t-t_o))$$

$$+ \frac{1}{\pi s_1} \int_{b'}^{\infty} \frac{1}{u} e^{-ut} [1-e^{ut_o} H(t-t_o)] \sin(\frac{u-b'}{D})^{1/2} s_1 \, du$$

$$+ \frac{1}{\pi s_2} \int_{b'}^{\infty} \frac{1}{u} e^{-ut} [1-e^{ut_o} H(t-t_o)] \sin(\frac{u-b'}{D})^{1/2} s_2 \, du\}$$

$$(3.33)$$

where $s_1^2 = x^2+y^2+(z-h_s)^2$, $s_2^2 = x^2+y^2+(z+h_s)^2$.

It is noted that equations (3.30) and (3.31) can be obtained by the following relations :

$$C_2(x,y,z,t) = \int_0^t C_1(x,y,z,t')\,dt' \tag{3.34}$$

$$C_{p2}(x,y,z,t) = \int_0^t C_{p1}(x,y,z,t')\,dt' \tag{3.35}$$

and $W_o = W_c$.

It is found that equations (3.32) and (3.33) can also be derived by the following relations :

$$C_3(x,y,z,t) = \int_0^t C_1(x,y,z,t')dt' - H(t-t_o) \int_0^{t-t_o} C_1(x,y,z,t'-t_o)dt' \tag{3.36}$$

$$C_{p3}(x,y,z,t) = \int_0^t C_{p1}(x,y,z,t')dt' - H\,(t-t_o) \int_0^{t-t_o} C_{p1}(y,y,z,t'-t_o)dt' \tag{3.37}$$

and $W_o = W_c$.

When $k_r = 0.0$, $k_a = 0.0$, $k_b = 0.0$, the expressions for C and C_p in each case are same as obtained in Chapter II.

3.4 RESULTS AND DISCUSSION

To see the effect of various parameters on the concentration distribution of both the species in each case, we use following dimensionless quantities (As in Chapter II).

$$\bar{t} = \frac{D}{h_s^2}\,t\,,\ \bar{x} = \frac{x}{h_s}\,,\ \bar{y} = \frac{y}{h_s}\,,\ \bar{z} = \frac{z}{h_s}\,,$$

$$\bar{k} = \frac{h_s^2\,k}{D}\,,\ \bar{k}_g = \frac{k_g\,h_s^2}{D}\,,\ \bar{k}_p = \frac{k_p\,h_s^2}{D}\,,\ \bar{k}_a = \frac{k_a\,h_s^2}{D}$$

$$\bar{k}_b = \frac{k_b\,h_s^2}{D}\,,\ k_r = \frac{k_r\,h_s^2}{D}\,,\ \bar{U} = \frac{U\,h_s}{D}\,,\ \bar{C} = \frac{h_s\,D}{W_c}\,C\,,$$

$$\bar{C}_p = \frac{h_s\,D}{W_c}\,C_p\,,\ \bar{W}_o = \frac{W_o\,D}{W_c\,h_s^2}\,. \tag{3.38}$$

The concentration distribution for each case in dimensionless form can be written as (dropping bars for convenience) :

(i) Instantaneous flux

$$C_1(x,y,z,t) = \frac{W_o \exp(\frac{Ux}{2})}{(4\pi t)^{3/2}} \{\frac{b_2}{2M} e^{-b_1' t} [e^{-\frac{s_1^2}{4t}} + e^{-\frac{s_2^2}{4t}}]$$

$$+ \frac{b_3}{2M} e^{-b' t} [e^{-\frac{s_1^2}{4t}} + e^{-\frac{s_2^2}{4t}} \}] \qquad (3.39)$$

$$C_p(x,y,z,t) = \frac{W_o \exp(\frac{Ux}{2})}{(4\pi t)^{3/2}} \frac{k}{2M} \{e^{-b_1' t} [e^{-\frac{s_1^2}{4t}} + e^{-\frac{s_2^2}{4t}}]$$

$$- e^{-b' t} [e^{-\frac{s_1^2}{4t}} + e^{-\frac{s_2^2}{4t}}]\} \qquad (3.40)$$

where m′ and n′ in dimensionless forms are

$$m' = \frac{U^2}{4} + k + k_g + k_a$$

$$n' = \frac{U^2}{4} + k_r + k_b + k_p$$

$$s_1^2 = x^2+y^2+(z-1)^2 \ , \ s_2^2 = x^2+y^2+(z+1)^2 .$$

(ii) Constant flux

$$C_2(x,y,z,t) = \int_0^t C_1(x,y,z,t')\, dt' \qquad (3.41)$$

$$C_{p2}(x,y,z,t) = \int_0^t C_{p1}(x,y,z,t')\, dt' \qquad (3.42)$$

(iii) Step function type flux

$$C_3(x,y,z,t) = \int_0^t C_1(x,y,z,t')dt' - H(t-t_o) \int_0^{t-t_o} C_1(x,y,z,t'-t_o)dt' \quad (3.43)$$

$$C_{p3}(x,y,z,t) = \int_0^t C_{p1}(x,y,z,t')dt' - H(t-t_o) \int_0^{t-t_o} C_{p1}(x,y,z,t'-t_o)dt' \quad (3.44)$$

The dimensionless concentration distributions of C and C_p at the ground level have been computed and depicted in figs. (3.1-3.9) for each case and for different values of k, k_r, t, $U = 5.0$, $W_o = 1.0$ and $k_a = k_b = k_g = k_p = 0.0$. It is found that C is greater than C_p when $k = 1.0$, $k_r = 10.0$ in each case (see figs. 3.1 - 3.3) but reverse is the situation when $k_r = 1.0$, $k = 10.0$ (see figs. 3.4 - 3.6). However, when $k_r=k=1.0$ (see fig. 3.7-3.9), the concentrations C and C_p tend to their equal equilibrium values as downwind distance increases after particular time.

To see the effects of removal rate parameters on C and C_p, the expressions given by equations (3.39) - (3.44) are computed and plotted in figs. (3.10 - 3.12), for following set of parameters : $U = 5.0$, $W_o = 1.0$, $k = 1.0$, $k_r = 1.0$, $k_a = 0.005$, $k_g = 0.05$, $k_b = 0.002$, $k_p = 0.05$, $z = 0.0$, $y = 0.0$. It is seen from these figs. that the concentrations C and C_p decrease as removal parameters increase. Also from these figs. (3.10 - 3.12), the following remarks can be made as pointed out in Chapter II.

(i) When the flux is instantaneous, it is noted from fig. 3.10 that as time increases the concentrations of both the species decrease and the point of maxima in the concentration distance profile of both the species moves away from the source.

(ii) In the case of constant flux (see fig. 3.11) it is seen that the concentrations of both the species increase as time increases and reach to their respective steady state values.

(iii) For the step function type flux, it is observed that the concentrations of both the species decrease as time increases for $t > t_o$. However for $t \leq t_o$ the profiles for C and C_p will be similar to the case of constant flux.

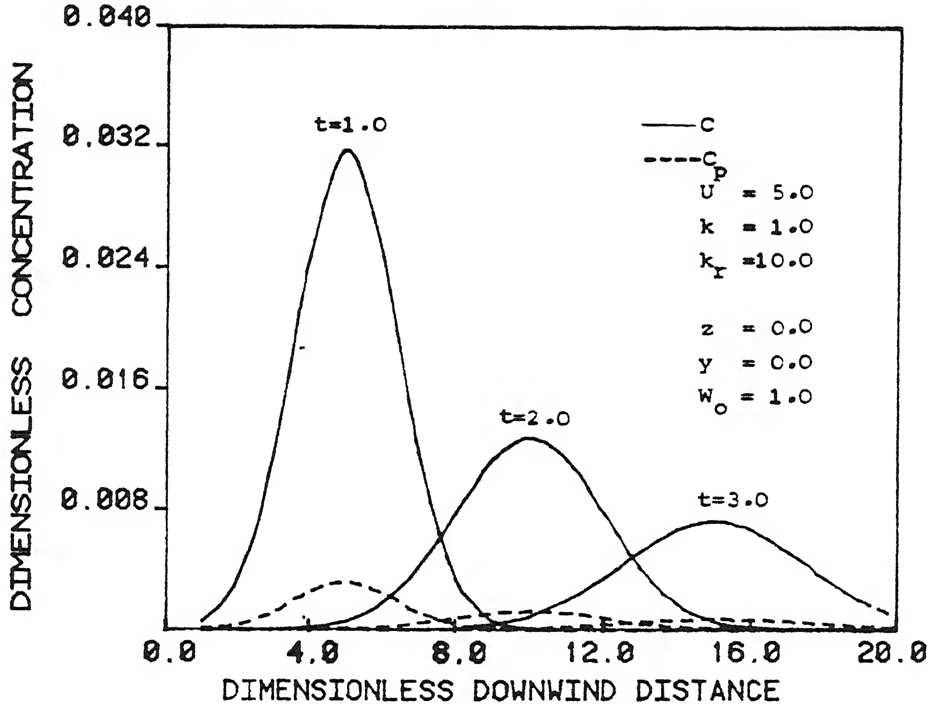


FIG 3.1 FLUX IS INSTANTANEOUS AT THE SOURCE

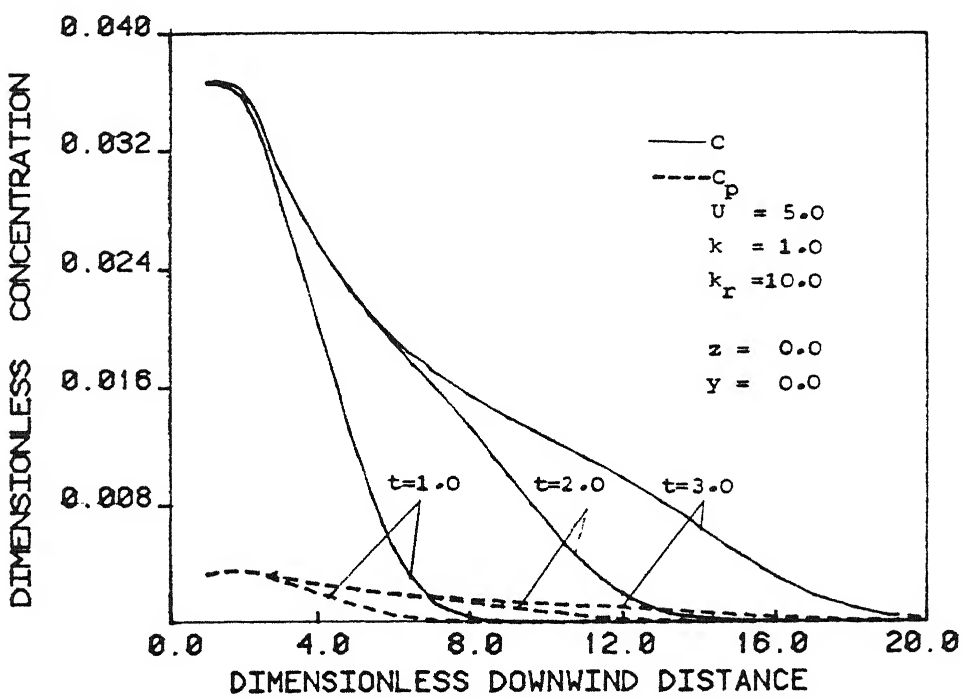


FIG 3.2 FLUX IS CONSTANT AT THE SOURCE

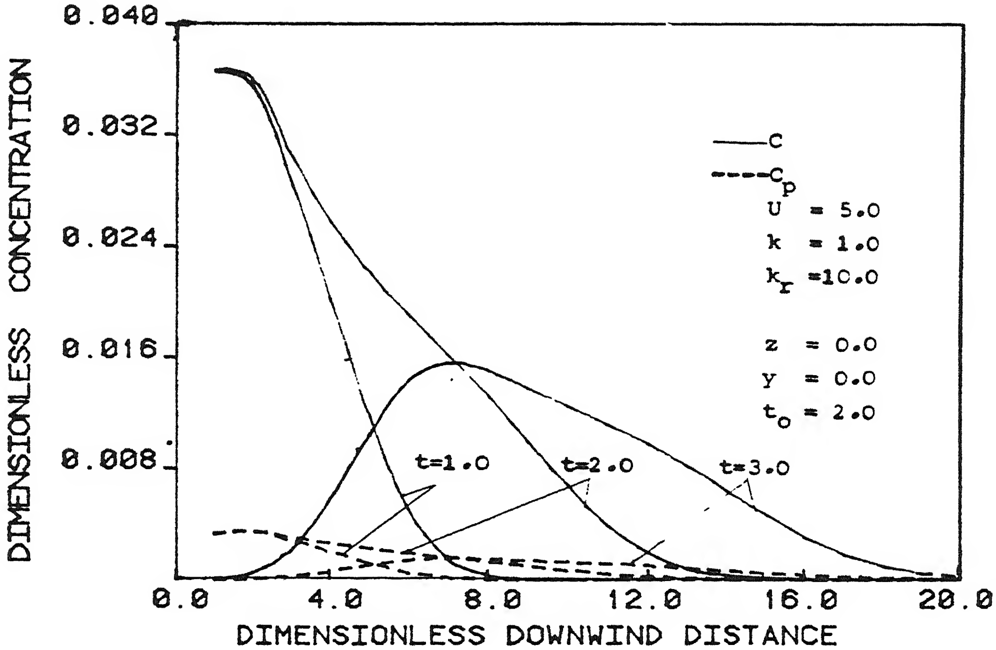


FIG3.3 FLUX IS STEP FUNCTION TYPE AT THE SOURCE

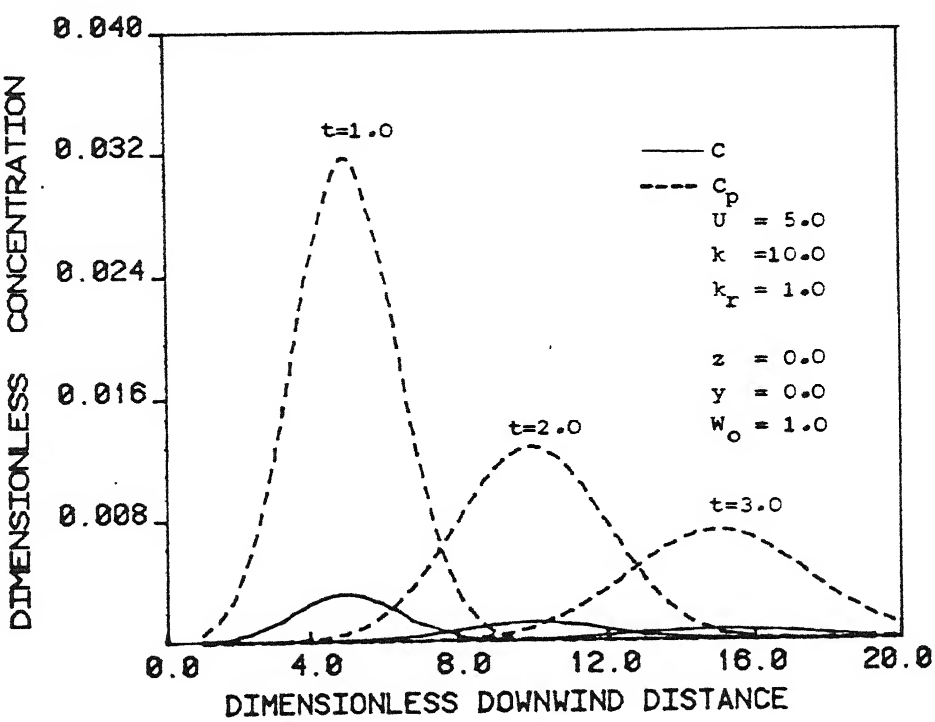


FIG3.4 FLUX IS INSTANTANEOUS AT THE SOURCE

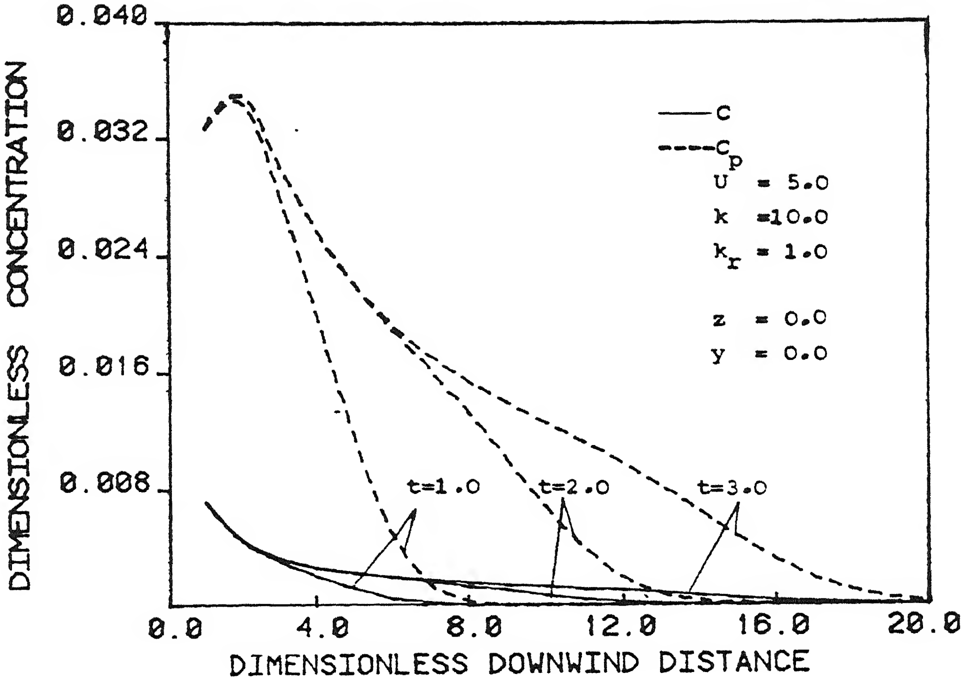


FIG3.5 FLUX IS CONSTANT AT THE SOURCE

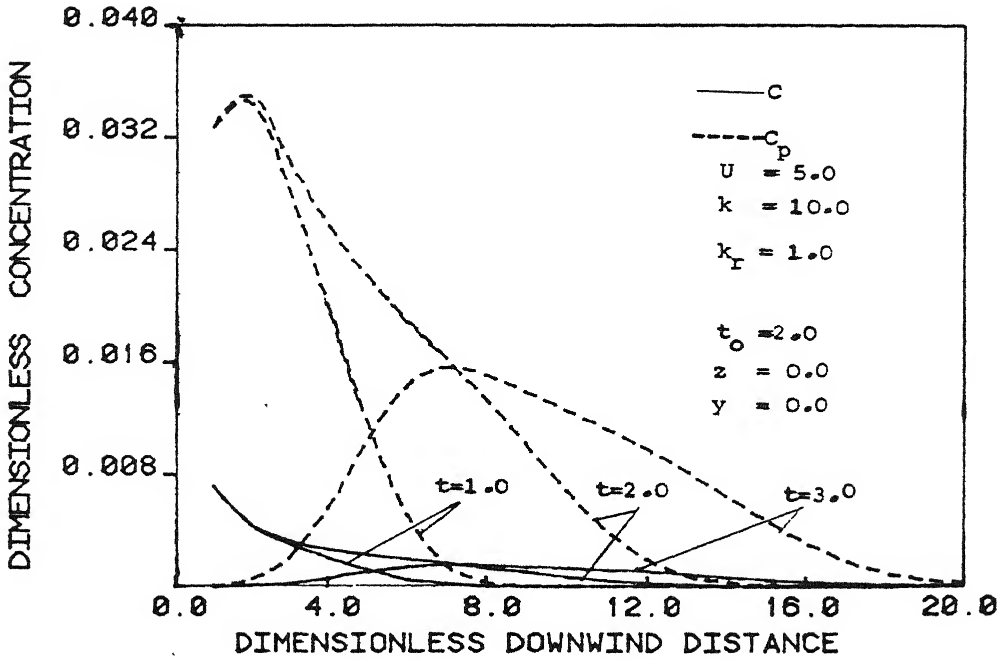


FIG3.6 FLUX IS STEP FUNCTION TYPE AT THE SOURCE

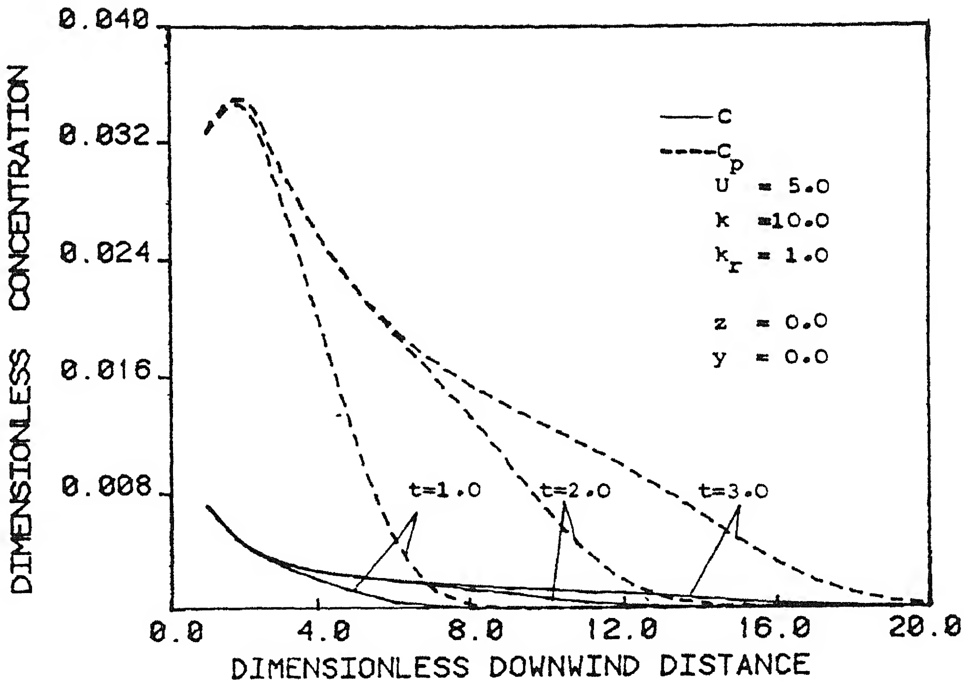


FIG3.5 FLUX IS CONSTANT AT THE SOURCE

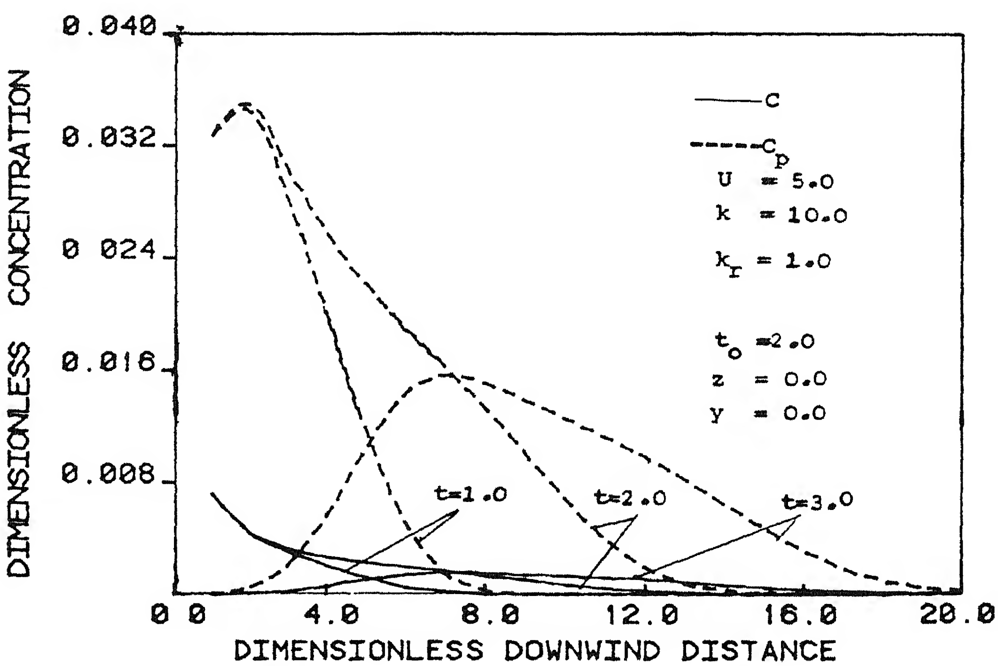


FIG3.6 FLUX IS STEP FUNCTION TYPE AT THE SOURCE

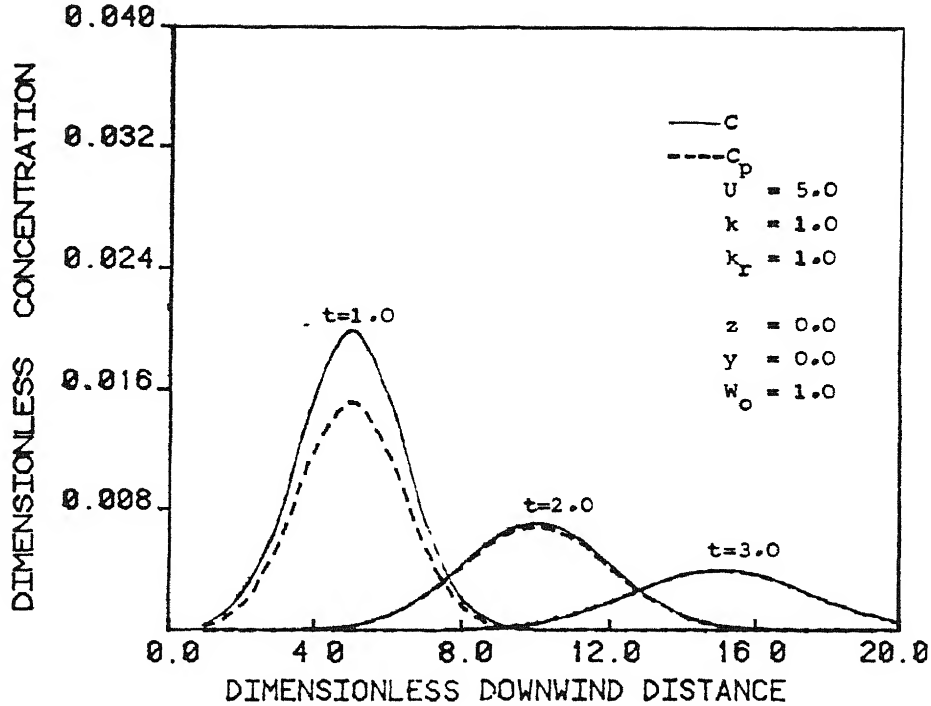


FIG 3.7 FLUX IS INSTANTANEOUS AT THE SOURCE

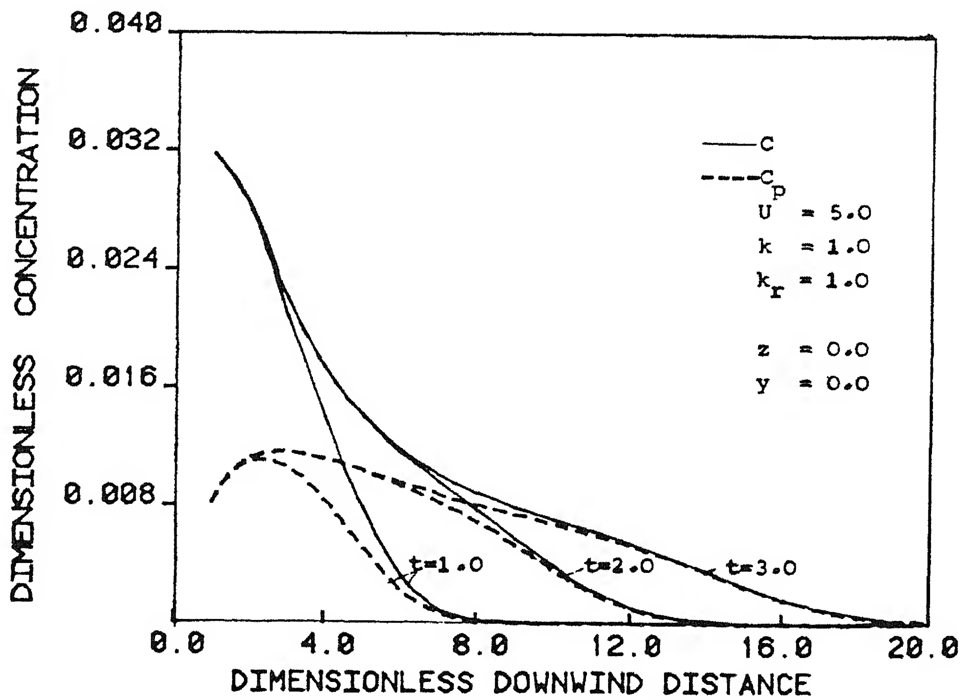


FIG3.8 FLUX IS CONSTANT AT THE SOURCE

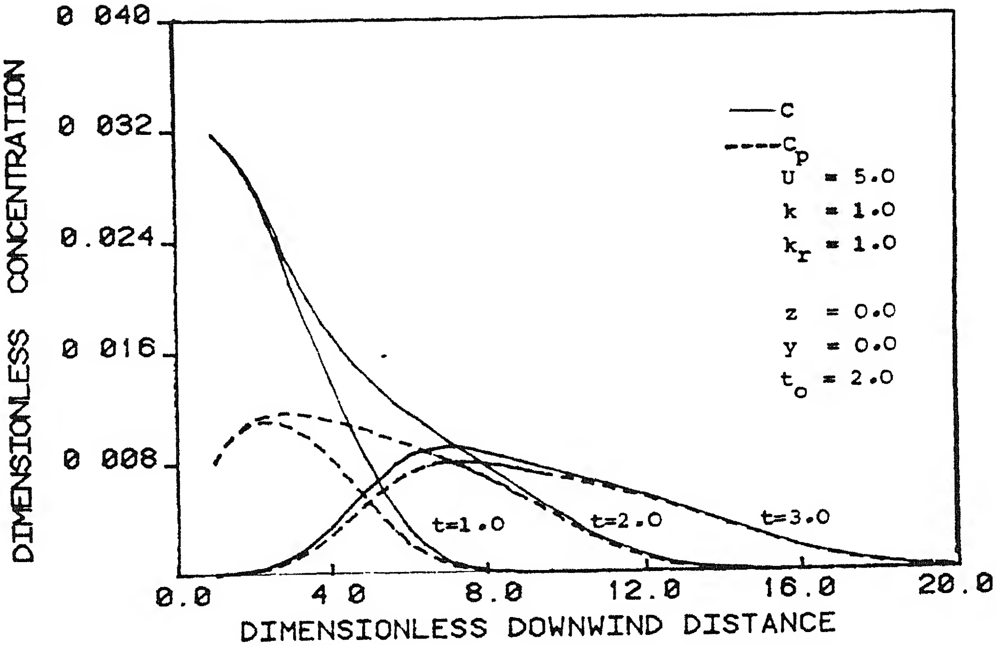


FIG3.9 FLUX IS STEP FUNCTION TYPE AT THE SOURCE

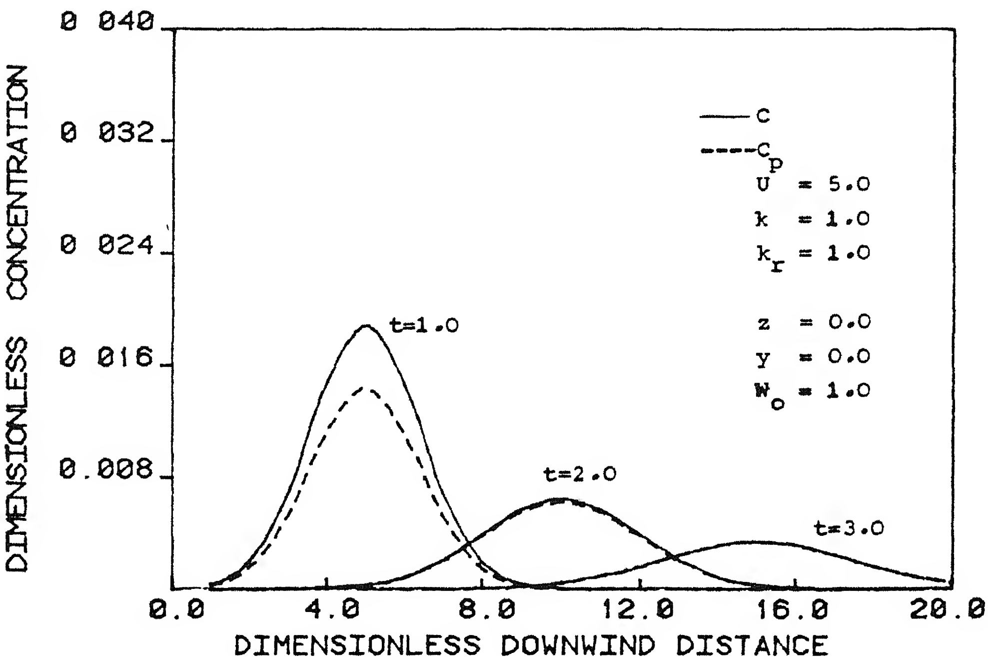


FIG3.10 FLUX IS INSTANTANEOUS AT THE SOURCE

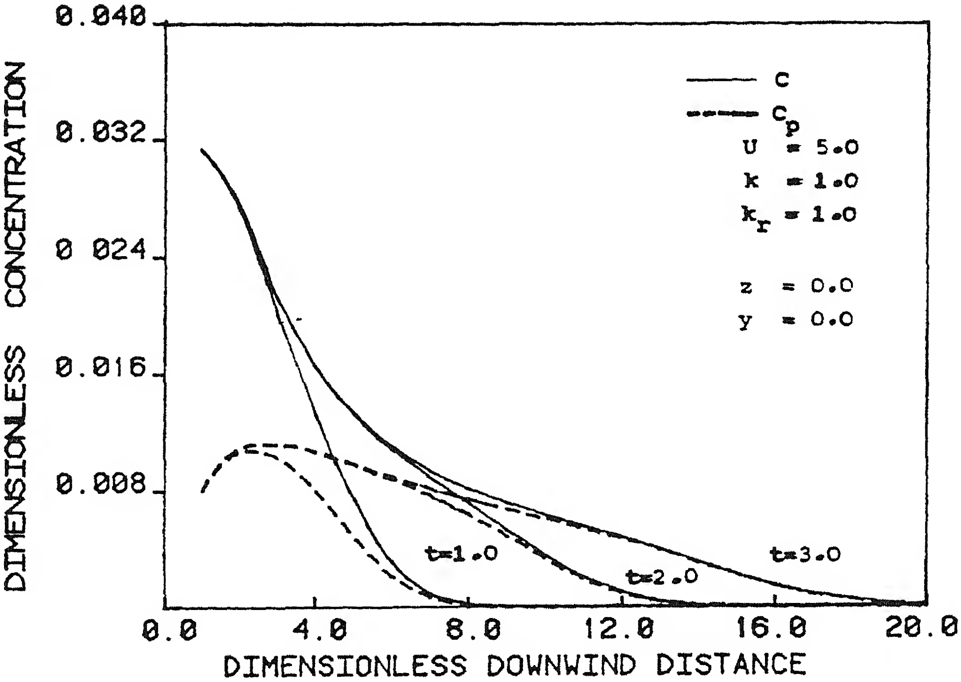


FIG 3.11 FLUX IS CONSTANT AT THE SOURCE

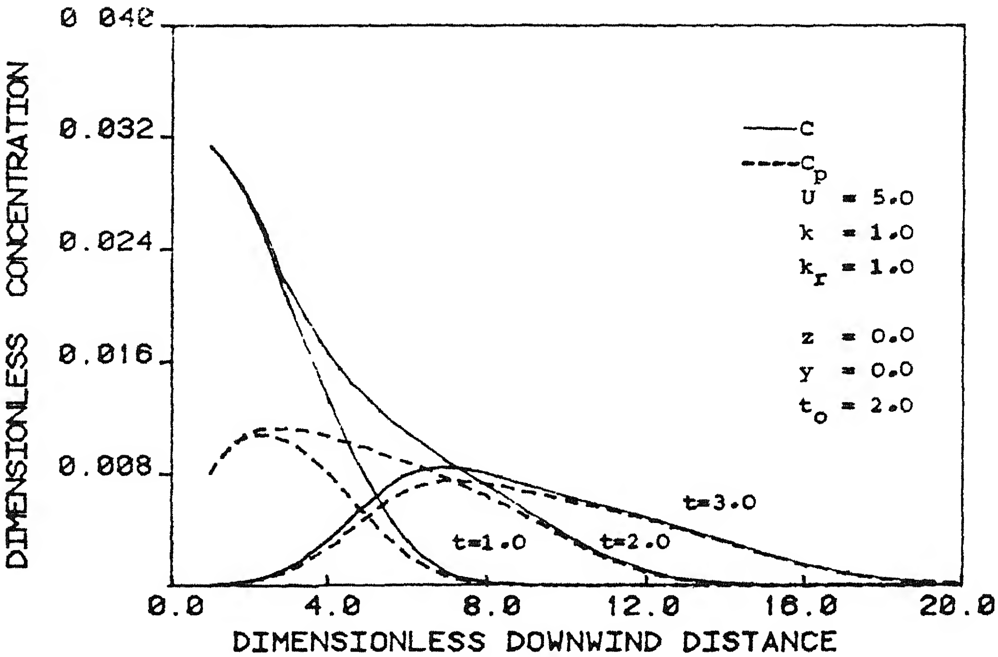


FIG 3.12 FLUX IS STEP FUNCTION TYPE AT THE SOURCE

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CHAPTER IV

DISPERSION OF A REACTIVE POLLUTANT FROM A TIME DEPENDENT POINT SOURCE FORMING SECONDARY POLLUTANT : WITHOUT INVERSION CONDITION

4.1 INTRODUCTION

As pointed out earlier the dispersion of air pollutant in atmosphere from a point source is governed by the process of molecular diffusion and convection and depends upon factors such as stack height, wind velocity, temperature inversion, dry deposition, rainout/washout, etc. (Pasquill, 1962; Seinfeld, 1975; Dobbins, 1979; Novotny and Chesters, 1981). Various investigations have been carried out to understand the dispersion of air pollutant by considering some of the above mentioned factors (Smith, 1957; Pasquill, 1962; Heines and Peters, 1973a, 1973b; Lamb and Seinfeld, 1973; Ermak, 1977; Peterson and Seinfeld, 1977; Karamchandani and Peters, 1983). Effects of removal by chemical reaction, rainout/washout etc. on the dispersal process have been studied by considering them as first order processes (Slinn, 1974, 1980; Scriven and Fisher, 1975; Nordlund,1975; Sander and Seinfeld, 1976; Prahm et al., 1976; McMohan et al., 1976; Sheih, 1977; Calvert et al., 1978; Peterson and Seinfeld, 1977; Alam and Seinfeld, 1981; Hales, 1982). In particular, Alam and Seinfeld (1981) have studied the dispersion of sulfur dioxide and sulfate from a point source by solving the steady state three dimensional diffusion equation

the secondary pollutant disperses in the same manner into the atmosphere as the primary species. The wind speed is assumed to be sufficiently large so that diffusive transport in the wind direction can be neglected in comparison to advection.

The unsteady state diffusion equation governing the concentration C for the gaseous pollutant can be written as follows :

$$\frac{\partial C}{\partial t} + U \frac{\partial C}{\partial x} - w \frac{\partial C}{\partial z} = K_y \frac{\partial^2 C}{\partial y^2} + K_z \frac{\partial^2 C}{\partial z^2} - (k+k_g)C \qquad (4.1)$$

where x axis is taken along the wind direction, z towards height, U is the mean wind velocity and K_y, K_z are diffusivity coefficients in y-, z-directions respectively. The constant k is the rate of conversion of primary species to secondary pollutant, k_g is its removal rate by some other mechanism (say washout) and w is the settling velocity.

The initial and boundary conditions for (4.1) are

$$C(x,y,z,t) = 0 \quad \text{at } t = 0 \quad x,y,z > 0 \qquad (4.2)$$

$$C(x,y,z,t) = \frac{W(t)}{U} \; \delta(y)\, \delta(z-h_s) \quad \text{at } x = 0 \qquad (4.3)$$

$$C(x,y,z,t) = 0 \quad \text{as } y \to \pm\infty, \quad t \geq 0 \qquad (4.4)$$

$$K_z \frac{\partial C}{\partial z} + wC = v_d\, C \text{ at } z = 0 \quad , \; t \geq 0 \qquad (4.5)$$

$$C = 0 \quad \text{as } z \to \infty \quad t \geq 0 \qquad (4.6)$$

where v_d is deposition velocity of the gaseous pollutant on the ground. The boundary condition (4.3) implies that the concentration has been prescribed at the source in terms of time dependent flux W(t). The following forms of W(t) are considered in the analysis :

(i) Instantaneous source,

$$W(t) = W_o\ \delta(t)$$

(ii) Constant source,

$$W(t) = W_c \quad \text{(constant)} \tag{4.7}$$

(iii) Step function type source,

$$\begin{aligned} W(t) &= W_c \qquad 0 < t \leq t_o \\ &= 0 \qquad\quad t > t_o \end{aligned}$$

where t_o is the duration of release of the gaseous pollutant from the source.

Similarly the differential equation governing the concentration C_p of the secondary pollutant can be written as

$$\frac{\partial C_p}{\partial t} + U \frac{\partial C_p}{\partial x} - w \frac{\partial C_p}{\partial z} = K_y \frac{\partial^2 C_p}{\partial y^2} + K_z \frac{\partial^2 C_p}{\partial z^2} + kC - k_p\ C_p \tag{4.8}$$

where k_p is its rate of removal.

If there is no direct emission of secondary pollutant from the source then the initial and boundary conditions for C_p are

$$C_p(x,y,z,t) = 0 \quad \text{at} \quad t = 0 \tag{4.9}$$

$$C_p(x,y,z,t) = 0 \qquad \text{at } x = 0 \qquad t \geq 0 \tag{4.10}$$

$$C_p(x,y,z,t) = 0 \qquad \text{as } y \to \pm\infty \qquad t \geq 0 \tag{4.11}$$

$$K_z \frac{\partial C_p}{\partial z} + wC_p = v_{d_p} C_p \qquad \text{as } z = 0 \qquad t \geq 0 \tag{4.12}$$

$$C_p = 0 \qquad \text{as } z \to \infty \qquad t \geq 0 \tag{4.13}$$

where v_{d_p} is deposition velocity of secondary pollutant on the ground.

Using the following dimensionless variables

$$\bar{t} = \frac{K_z t}{h_a^2}, \quad \bar{x} = \frac{K_z x}{U h_a^2}, \quad \bar{y} = \frac{y}{h_a}, \quad \bar{z} = \frac{z}{h_a}, \quad \bar{h}_s = \frac{h_s}{h_a} \tag{4.14}$$

$$\bar{C} = \frac{U h_a^2}{W_c} C, \quad \bar{C}_p = \frac{U h_a^2 C_p}{W_c}, \quad \bar{w} = \frac{w h_a}{K_z}, \quad \bar{W}_o = \frac{W_o h_a^2}{W_c K_z}, \quad \bar{W}(t) = \frac{W(t)}{W_c},$$

equations (4.1)-(4.13) can be written in the dimensionless form as (dropping bars for convenience)

$$\frac{\partial C}{\partial t} + \frac{\partial C}{\partial x} - w \frac{\partial C}{\partial z} = \beta \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2} - (\alpha + \alpha_g)C \tag{4.15}$$

$$C(x,y,z,t) = 0 \qquad \text{at } t = 0 \tag{4.16}$$

$$C(x,y,z,t) = W(t)\, \delta(y)\, \delta(z-h_s) \qquad \text{at } x = 0 \tag{4.17}$$

$$C(x,y,z,t) = 0 \qquad \text{as } y \to \pm\infty \tag{4.18}$$

$$\frac{\partial C}{\partial z} + wC = NC \qquad \text{at } z = 0 \tag{4.19}$$

$$C = 0 \qquad \text{as } z \to \infty \tag{4.20}$$

(i) $W(t) = W_o\ \delta(t)$

(ii) $W(t) = 1$ (4.21)

(iii) $W(t) = 1 \qquad 0 \leq t \leq t_o$

$\qquad = 0 \qquad t > t_o$

$$\frac{\partial C_p}{\partial t} + \frac{\partial C_p}{\partial x} - w\frac{\partial C_p}{\partial z} = \beta\frac{\partial^2 C_p}{\partial y^2} + \frac{\partial^2 C_p}{\partial z^2} + \alpha C - \alpha_p\ C_p \tag{4.22}$$

$$C_p(x,y,z,t) = 0 \quad \text{at } t = 0 \tag{4.23}$$

$$C_p(x,y,z,t) = 0 \quad \text{at } x = 0 \tag{4.24}$$

$$C_p(x,y,z,t) = 0 \quad \text{as } y \to \pm\infty \tag{4.25}$$

$$\frac{\partial C_p}{\partial z} + w\ C_p = N_p\ C_p \quad \text{at } z = 0 \tag{4.26}$$

$$C_p = 0 \qquad \text{as } z \to \infty \tag{4.27}$$

where

$$\beta = \frac{K_y}{K_z}\ ,\ \alpha = \frac{k\ h_a^2}{K_z}\ ,\ \alpha_g = \frac{k_g\ h_a^2}{K_z}\ ,\ N = \frac{v_d\ h_a}{K_z}$$

$$\alpha_p = \frac{k_p\ h_a^2}{K_z}\ ,\ N_p = \frac{v_{d_p}\ h_a}{K_z}$$

and h_a is some characteristic height chosen as source height.

4.3 METHOD OF SOLUTION

Equations (4.15) and (4.22) can be written in the compact form as

$$L \begin{bmatrix} C \\ C_p \end{bmatrix} - \begin{bmatrix} \alpha+\alpha_g & 0 \\ -\alpha & \alpha_p \end{bmatrix} \begin{bmatrix} C \\ C_p \end{bmatrix} = 0 \tag{4.28}$$

where $L = -\frac{\partial}{\partial t} - \frac{\partial}{\partial x} + w\frac{\partial}{\partial z} + \beta\frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ is an operator.

Using the same transform (see Astarita et al., (1979), Alam and Seinfeld (1981), Chapter II), we get uncoupled system

$$LC - (\alpha + \alpha_g)\, C = 0 \tag{4.29}$$

$$LB - \alpha_p\, B = 0 \tag{4.30}$$

where $B = C_p - \frac{\alpha C}{\alpha_p - \alpha - \alpha_g}$.

The corresponding conditions for B are,

$$B(x,y,z,t) = 0 \quad \text{at } t = 0 \tag{4.31}$$

$$B(x,y,z,t) = \frac{-\alpha}{\alpha_p - \alpha - \alpha_g} W(t)\, \delta(y)\, \delta(z-h_s) \text{ at } x = 0 \tag{4.32}$$

$$B(x,y,z,t) = 0 \quad \text{as } y \to \pm\infty \tag{4.33}$$

$$\frac{\partial B}{\partial z} + wB = N_p B + \frac{(N_p - N)\alpha C}{(\alpha_p - \alpha - \alpha_g)} \text{ at } z = 0 \tag{4.34}$$

$$B = 0 \quad \text{as} \quad z \to \infty \tag{4.35}$$

Assuming that the solutions of equations (4.29) and (4.30) are of the following forms

$$\begin{aligned} C &= C_1\, e^{-\frac{w}{2}(z-h_s) - \frac{w^2}{4}x} \\ B &= B_1\, e^{-\frac{w}{2}(z-h_s) - \frac{w^2}{4}x} \end{aligned} \tag{4.36}$$

we have,

$$\frac{\partial C_1}{\partial t} + \frac{\partial C_1}{\partial x} = \beta \frac{\partial^2 C_1}{\partial y^2} + \frac{\partial^2 C_1}{\partial z^2} - (\alpha + \alpha_g) C_1 \tag{4.37}$$

$$\frac{\partial B_1}{\partial t} + \frac{\partial B_1}{\partial x} = \beta \frac{\partial^2 B_1}{\partial y^2} + \frac{\partial^2 B_1}{\partial z^2} - \alpha_p B_1 \tag{4.38}$$

$$C_1 = 0, \quad t = 0, \; y \to \pm\infty, \; z \to \infty \tag{4.39}$$

$$B_1 = 0, \quad t = 0 \quad y \to \pm\infty, \; z \to \infty \tag{4.40}$$

$$C_1 = W(t)\, \delta(y)\, \delta(z-h_s) \quad e^{\frac{W}{2}(z-h_s)} \quad \text{at } x = 0 \tag{4.41}$$

$$B_1 = -\frac{\alpha}{(\alpha_p-\alpha-\alpha_g)} W(t)\, \delta(y)\, \delta(z-h_s) \quad e^{\frac{W}{2}(z-h_s)} \text{at } x = 0 \tag{4.42}$$

$$\frac{\partial C_1}{\partial z} = (N - \frac{W}{2}) C_1 \quad \text{at } z = 0 \tag{4.43}$$

$$\frac{\partial B_1}{\partial z} = (N_p - \frac{W}{2}) B_1 + \frac{\alpha(N_p-N)C_1}{(\alpha_p-\alpha-\alpha_g)} \text{ at } z = 0. \tag{4.44}$$

The solutions for both C_1 and B_1 are obtained by using Laplace and Fourier transforms in each case and finally we have

(i) For instantaneous source

$$C_1(x,y,z,t) = W_o\, P(x,y,z)\, \delta(t-x) \tag{4.45}$$

$$B_1(x,y,z,t) = W_o\, Q(x,y,z)\, \delta(t-x) \tag{4.46}$$

where

$$P(x,y,z) = \frac{\exp(-y^2/4\beta x)}{4\pi\sqrt{\beta}\, x} e^{-(\alpha+\alpha_g)x} \left[\{ e^{\frac{-(z-h_s)^2}{4x}} + \right.$$

$$e^{-\frac{(z+h_s)^2}{4x}\}} - (4\pi x)^{1/2} \ (N - \tfrac{W}{2}) \ e^{(N-\frac{W}{2})^2 x + (N - \frac{W}{2})(z+h_s)}$$

$$\times \ \mathrm{erfc}\ \{\frac{z+h_s}{2\sqrt{x}} + (N - \tfrac{W}{2})x^{1/2}\}]$$

$$Q(x,y,z) = \frac{\alpha}{\alpha_p - \alpha - \alpha_g} \ \frac{\exp(-\frac{y^2}{4\beta x})}{2\sqrt{\pi\beta x}} \ e^{-\alpha_p x}$$

$$[(N-N_p) \int_0^x e^{-(\alpha+\alpha_g-\alpha_p)x'} \ \frac{1}{\sqrt{4\pi x'}} \ \{2e^{\frac{-h_s^2}{4x'}}$$

$$-(4\pi x')^{1/2}(N-\tfrac{W}{2})e^{(N-\frac{W}{2})^2 \ x' + (N-\frac{W}{2})h_s} \ \mathrm{erfc}(\frac{h_s}{2\sqrt{x'}} + (N-\tfrac{W}{2})\sqrt{x'})\} \ \times$$

$$\{\frac{1}{\sqrt{\pi(x-x')}} e^{\frac{-z^2}{4(x-x')}} - (N_p - \tfrac{W}{2}) \ e^{(N_p - \frac{W}{2})z + (N_p - \frac{W}{2})^2 (x-x')} \qquad \times$$

$$\mathrm{erfc}\ (\frac{z}{2\sqrt{x-x'}} + (N_p - \tfrac{W}{2})(x-x')^{1/2})\}dx' - \frac{1}{\sqrt{4\pi x}} \{(e^{\frac{-(z-h_s)^2}{4x}} \quad +$$

$$e^{\frac{-(z+h_s)^2}{4x}}) - (4\pi x)^{1/2} \ (N_p - \tfrac{W}{2})e^{(N_p - \frac{W}{2})^2 x + (N_p - \frac{W}{2})(z+h_s)}$$

$$\mathrm{erfc}\ (\frac{z+h_s}{2\sqrt{x}} + (N_p - \tfrac{W}{2})x^{1/2})]$$

and Dirac delta function $\delta(t-x)$ is defined as (see Carslaw and Jaeger, 1941)

$$\begin{aligned} \delta(t-x) &= 0 & & t < x \\ &= \frac{1}{\varepsilon} & & x \le t \le x+\varepsilon \\ &= 0 & & t > x+\varepsilon \end{aligned}$$

(ii) For constant source

$$C_1 = P(x,y,z)\ H(t-x) \tag{4.47}$$

$$B_1 = Q(x,y,z)\ H(t-x) \tag{4.48}$$

where $H(t-x)$ is Heaviside function defined as (Carslaw and Jaeger, 1941)

$$\begin{aligned} H(t-x) &= 0 && t \leq x \\ &= \frac{t}{x+\varepsilon} && x < t \leq x+\varepsilon \\ &= 1 && t > x+\varepsilon \end{aligned} \tag{4.49}$$

(iii) For step function type source

$$C_1 = P(x,y,z)\left[H(t-x)-H(t-t_o-x)\ H(t-t_o)\right] \tag{4.50}$$

$$B_1 = Q(x,y,z)\left[H(t-x)-H(t-t_o-x)\ H(t-t_o)\right] \tag{4.51}$$

It is found that as $t_o \rightarrow \infty$ equations (4.50) and (4.51) reduce to (4.47) and (4.48) respectively.

Finally using (4.36), the solutions for $C(x,y,z,t)$ and $B(x,y,z,t)$ in each case can be written as follows :

(i) For instantaneous source

$$C(x,y,z,t) = W_o\ P(x,y,z)\ \delta(t-x)e^{-\frac{W}{2}(z-h_s)-\frac{W^2}{4}x} \tag{4.52}$$

$$B(x,y,z,t) = W_o\ Q(x,y,z)\ \delta(t-x)e^{-\frac{W}{2}(z-h_s)-\frac{W^2}{4}x} \tag{4.53}$$

(ii) For constant source

$$C(x,y,z,t) = P(x,y,z)\ H(t-x)\ e^{-\frac{W}{2}(z-h_s) - \frac{W^2}{4} x} \tag{4.54}$$

$$B(x,y,z,t) = Q(x,y,z)H(t-x)e^{-\frac{W}{2}(z-h_s) - \frac{W^2}{4} x} \tag{4.55}$$

It is noted here that if $\alpha = 0.0$, $\alpha_g = 0.0$ and $t \to \infty$ equation (4.54) reduces to same form as obtained by Ermak(1977).

(iii) For step function type source

$$C(x,y,z,t) = P(x,y,z)\ [H(t-x)-H(t-t_o-x)\ H(t-t_o)] \times$$
$$e^{-\frac{W}{2}(z-h_s) - \frac{W^2}{4}x} \tag{4.56}$$

$$B(x,y,z,t) = Q(x,y,z)\ [H(t-x)-H(t-t_o-x)H(t-t_o)] \times$$
$$e^{-\frac{W}{2}(z-h_s) - \frac{W^2}{4} x} \tag{4.57}$$

The dimensionless concentration C_p can be obtained from C and B in each of the above mentioned casesby the following relation

$$C_p(x,y,z,t) = B(x,y,zt) + \frac{\alpha C(x,y,z,t)}{(\alpha_p-\alpha-\alpha_g)} \tag{4.58}$$

4.4 CROSS WIND INTEGRATED SOLUTIONS FOR LINE SOURCE

In the case of **line** source, C and C_p can be obtained from the above solution in each case separately by integrating

C and C_p with respect to y between $-\infty$ to ∞. These are given as follows :

(i) For instantaneous source

$$C(x,z,t) = W_o\, P(x,z)\, \delta(t-x) \tag{4.59}$$

$$C_p(x,z,t) = B(x,z,t) + \frac{\alpha C(x,z,t)}{(\alpha_p-\alpha-\alpha_g)} \tag{4.60}$$

where

$$B(x,z,t) = W_o\, Q(x,z)\, \delta(t-x)$$

$$P(x,z) = \frac{1}{\sqrt{4\pi x}}\, e^{-(\alpha+\alpha_g+\frac{w^2}{4})x-\frac{w}{2}(z-h_s)}\, [\{e^{\frac{-(z-h_s)^2}{4x}} + e^{\frac{-(z+h_s)^2}{4x}}\}$$

$$-(4\pi x)^{1/2}(N-\tfrac{w}{2})e^{(N-\frac{w}{2})^2x+(N-\frac{w}{2})(z+h_s)}\, \mathrm{erfc}\{\frac{z+h_s}{2\sqrt{x}} + (N-\tfrac{w}{2})x^{1/2}\}]$$

$$Q(x,z) = \frac{\alpha}{(\alpha_p-\alpha-\alpha_g)}\, \exp\{-(\alpha_p+\frac{w^2}{4})x - \frac{w}{2}(z-h_s)\}$$

$$[(N-N_p)\int_0^x e^{-(\alpha+\alpha_g-\alpha_p)x'}\, \frac{1}{\sqrt{4\pi x'}}\, \{2\, e^{\frac{-h_s^2}{4x'}}$$

$$-(4\pi x')^{1/2}(N-\tfrac{w}{2})\, \exp\{(N-\tfrac{w}{2})^2\, x' + (N-\tfrac{w}{2})h_s\}$$

$$\times\, \mathrm{erfc}(\frac{h_s}{2\sqrt{x'}} + (N-\tfrac{w}{2})\sqrt{x'})\}\, \{\frac{1}{\sqrt{\pi(x-x')}}\, e^{\frac{-z^2}{4(x-x')}} -$$

$$(N_p-\tfrac{w}{2})e^{(N_p-\frac{w}{2})z+(N_p-\frac{w}{2})^2(x-x')}\, \mathrm{erfc}(\frac{z}{2\sqrt{x-x'}}$$

$$+ (N_p-\tfrac{w}{2})\sqrt{x-x'})\}\, dx'$$

$$- \frac{1}{\sqrt{4\pi x}} \{ e^{\frac{-(z-h_s)^2}{4x}} + e^{\frac{-(z+h_s)^2}{4x}} - (4\pi x)^{1/2} (N_p - \frac{W}{2}) \times$$

$$\exp\{ (N_p - \frac{W}{2})^2 x + (N_p - \frac{W}{2})(z+h_s)\} \operatorname{erfc}(\frac{(z+h_s)}{2\sqrt{x}} + (N_p - \frac{W}{2})\sqrt{x}) \}]$$

(ii) For constant source

$$C(x,z,t) = P(x,z)\, H(t-x) \tag{4.61}$$

$$C_p(x,z,t) = Q(x,z)\, H(t-x) + \frac{\alpha\, C(x,z,t)}{(\alpha_p - \alpha - \alpha_p)} \tag{4.62}$$

(iii) For step function type source

$$C(x,z,t) = P(x,z)\, [H(t-x) - H(t-t_o-x)\, H(t-t_o)] \tag{4.63}$$

$$C_p(x,z,t) = Q(x,z)\, [H(t-x) - H(t-t_o-x)\, H(t-t_o)] + \frac{\alpha\, C(x,z,t)}{(\alpha_p - \alpha - \alpha_g)} . \tag{4.64}$$

4.5 RESULTS AND DISCUSSION

The effect of various parameters on the unsteadv state concentrationsof both species along the central line (0,0,1) are shown in figs. (4.1 - 4.9) in all the cases and for different valuesof t, $W_o = 1.0$. $N = 0.4$, $N_p = 0.04$, $z = 1.0$, $h_s = 1.0$, $\beta = 1.0$ and $y = 0.0$. It is observed that the concentrations C and C_p decrease as downwind distance increases (see fig. 4.3). As α increases the concentration

C decreases but C_p increases in all cases at a particular time and location (see fig. no. 4.7). From these figures it is also noted that the effect of removal is to decrease the concentrations of both the species.

When the source strength is instantaneous the concentration distributions along the central line are shown in figs. (4.1 - 4.2) for different values of t, $W_o = 1.0$, $\alpha = 0.11$, $\alpha_g = 0.02$, 0.08 and $\alpha_p = 0.2$, 0.8. It is noted that as time increases both C, C_p decrease, C_p being less than C for all the set of parameters chosen in graphs (4.1 - 4.2).

When the source strength is constant, the central line concentrations of both species are plotted in figs. (4.3-4.4) for different values of t, $\alpha = 0.11$, $\alpha_g = 0.02$, 0.08 and $\alpha_p = 0.2$, 0.8, $w = 0.04$. From these figures, it is observed that the concentrations of both the species C, C_p increase as time increases and reach to their respective steady state values as $t \to \infty$. It is also noted that for $t < x$ the concentrations of both the species are zero implying that the pollutant front has not reached the point x as yet.

When the flux is given by step type function, the central line concentrations C and C_p decrease as time increases for $t > t_o$ (see figs. 4.5 - 4.6) and for $t \leq t_o$ the behaviour is similar as in the case of constant flux.

The effect of settling velocity on the unsteady state ground level concentration is also studied and it is found that

the concentrations of both primary and secondary species increase as settling velocity increases (see fig. 4.9 for the case of constant flux).

Similar results, as discussed above, have also been noted in the case of line source for all the three types of time dependent sources (graphs are not shown).

To see the effect of settling velocity and other removal mechanisms (chemical reaction, dry deposition) on the concentration distribution at different heights, the steady state vertical distributions of the primary species in the case of constant flux for both point and line sources are depicted in figs. (4.10 - 4.15). It is noted from figs. (4.10, 4.13) corresponding to point and line sources, that as settling velocity increases, the concentration at a point increases when it is located below the source height for a given x. However, the results are just the reverse for points located above the source height.

The effects of removal mechanisms on the vertical concentration distributions in the case of point and line sources are depicted in figs. (4.11, 4.12, 4.14, 4.15). It is noted that the concentration decreases as α increases in both the cases.

The effect of ground level deposition parameter is shown in figs. (4.12, 4.15). It is observed that as the ground level deposition parameter increases the vertical concentration decreases, the effect of deposition being more pronounced below the source height.

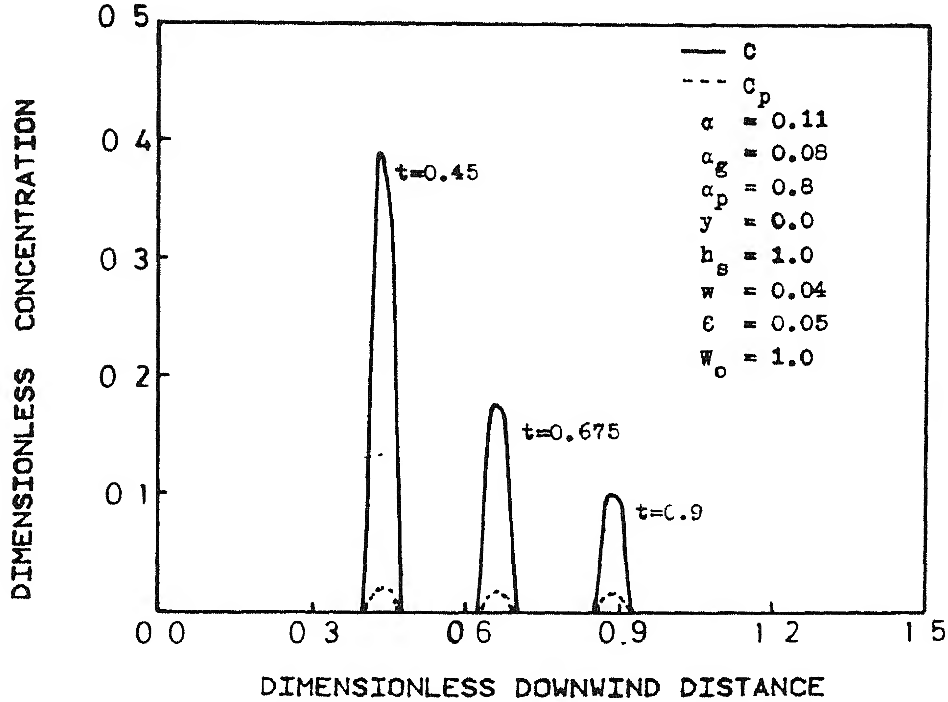


FIG 4.1 FLUX IS INSTANTANEOUS AT THE SOURCE

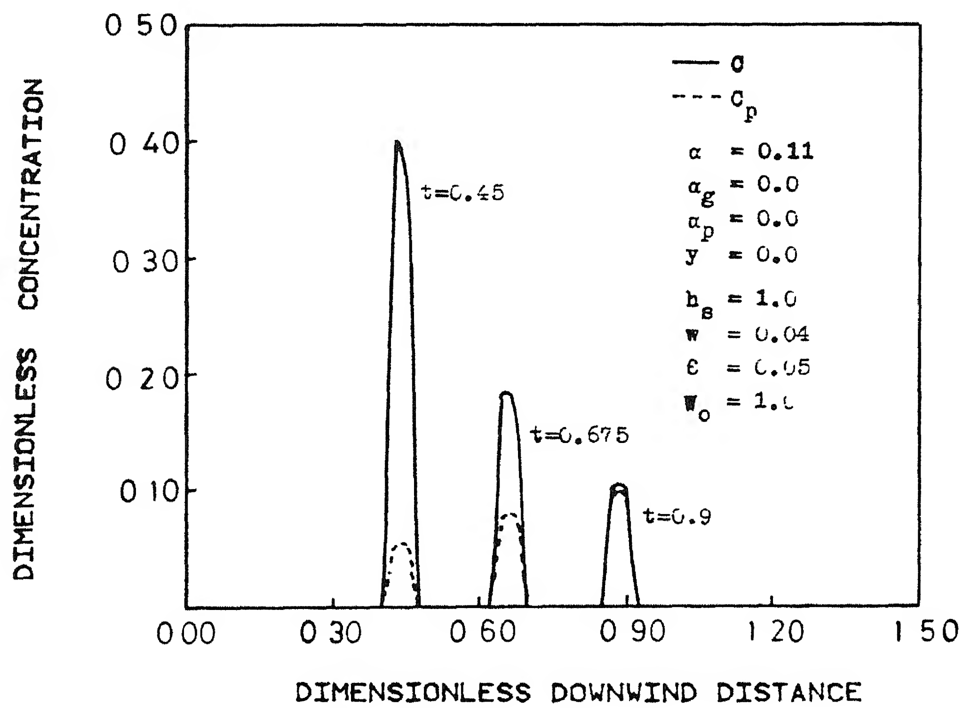


FIG 4.2 FLUX IS INSTANTANEOUS AT THE SOURCE

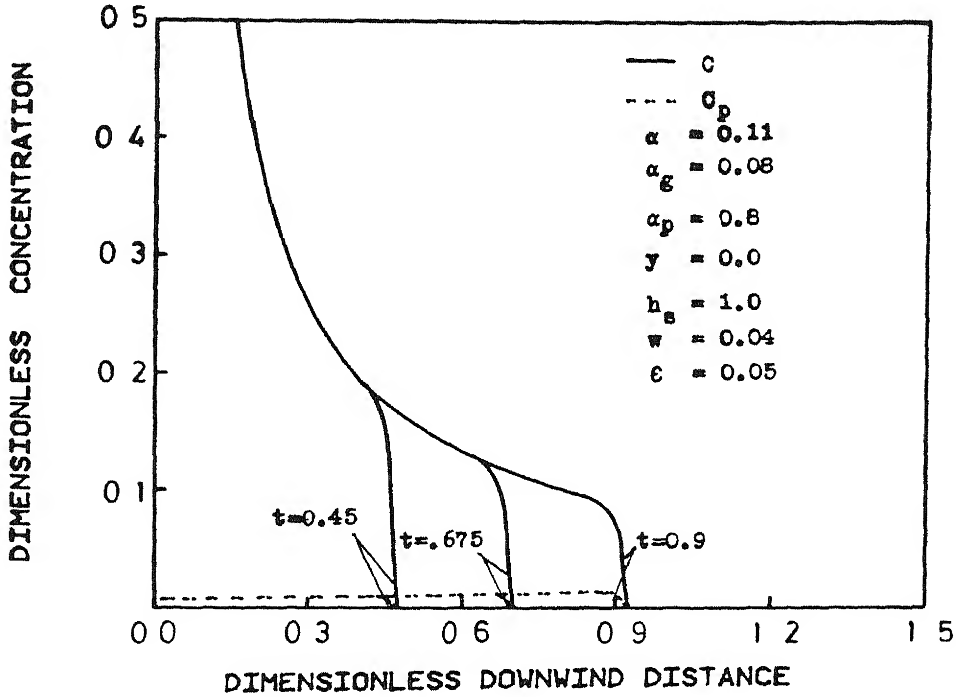


FIG 4.3 FLUX IS CONSTANT AT THE SOURCE

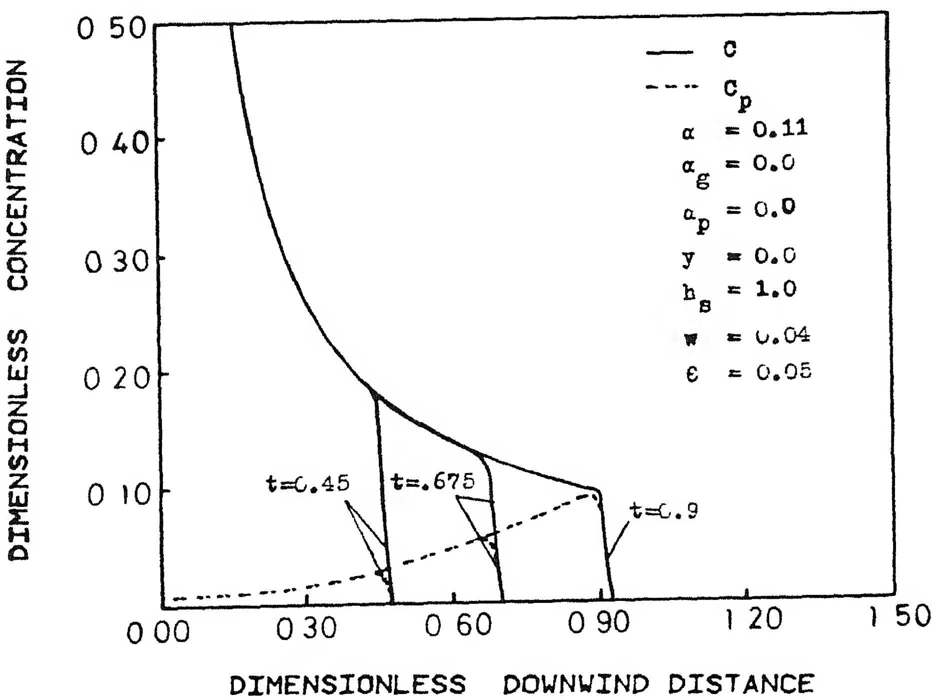
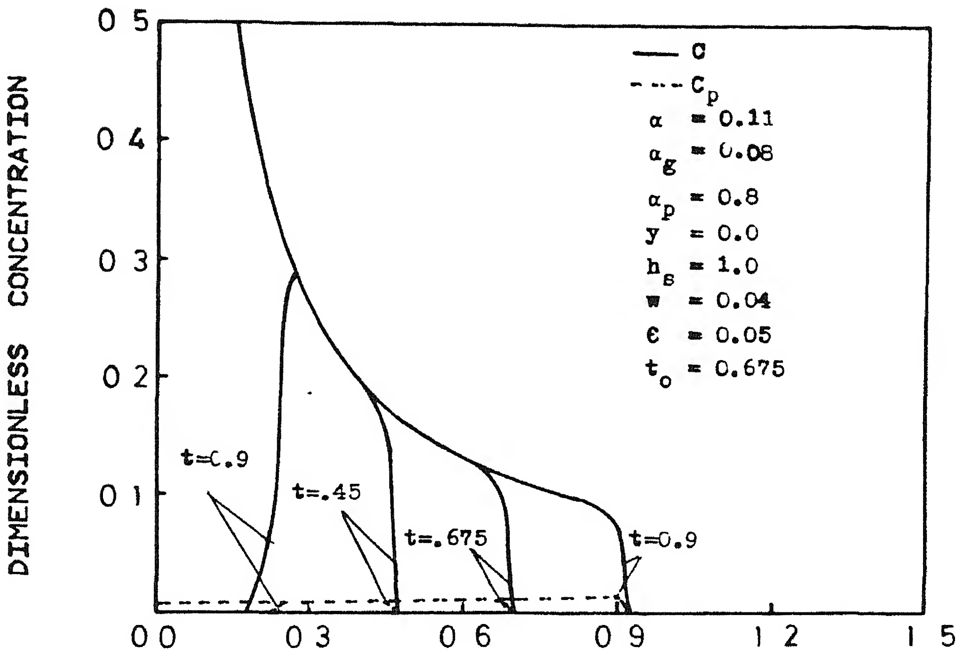
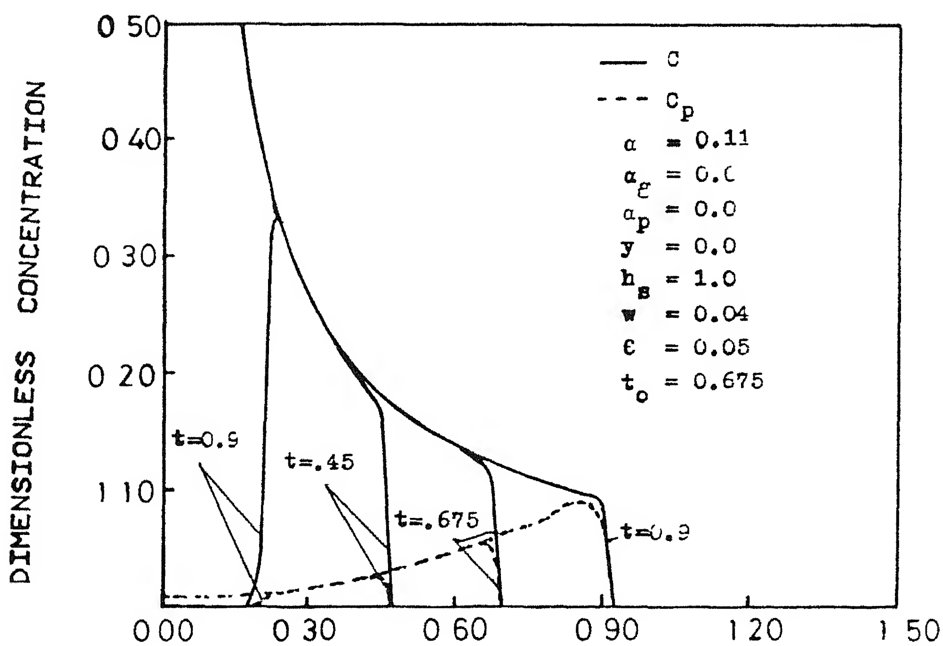


FIG 4.4 FLUX IS CONSTANT AT THE SOURCE



DIMENSION DOWNWIND DISTANCE

FIG 4 5 FLUX IS STEP FUNCTION TYPE AT THE SOURCE



DIMENSIONLESS DOWNWIND DISTANCE

FIG 4.6 FLUX IS STEP FUNCTION TYPE AT THE SOURCE

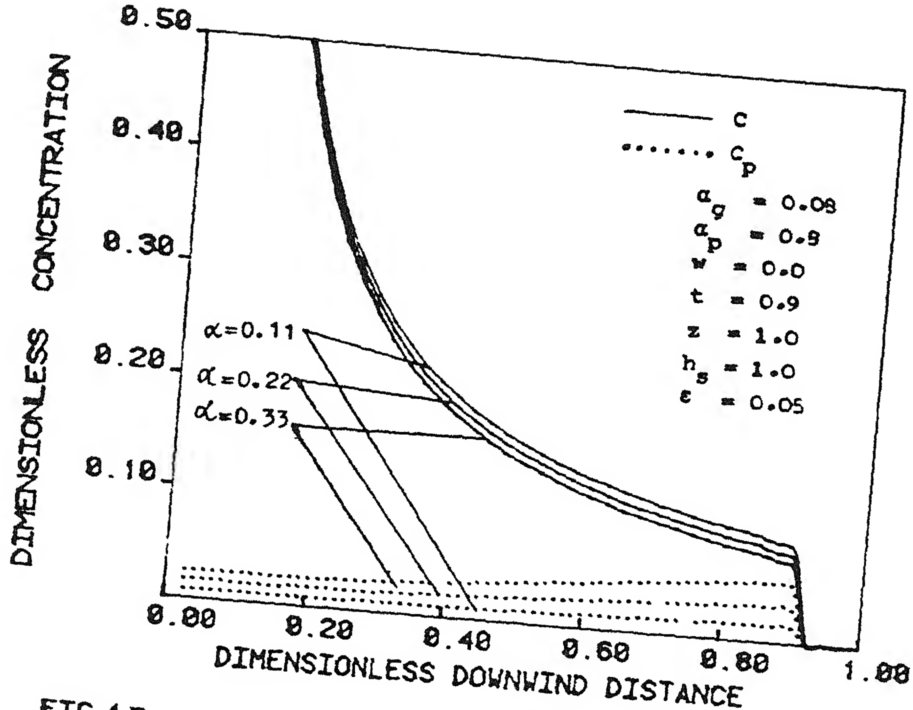


FIG 4.7 FLUX IS CONSTANT AT THE SOURCE

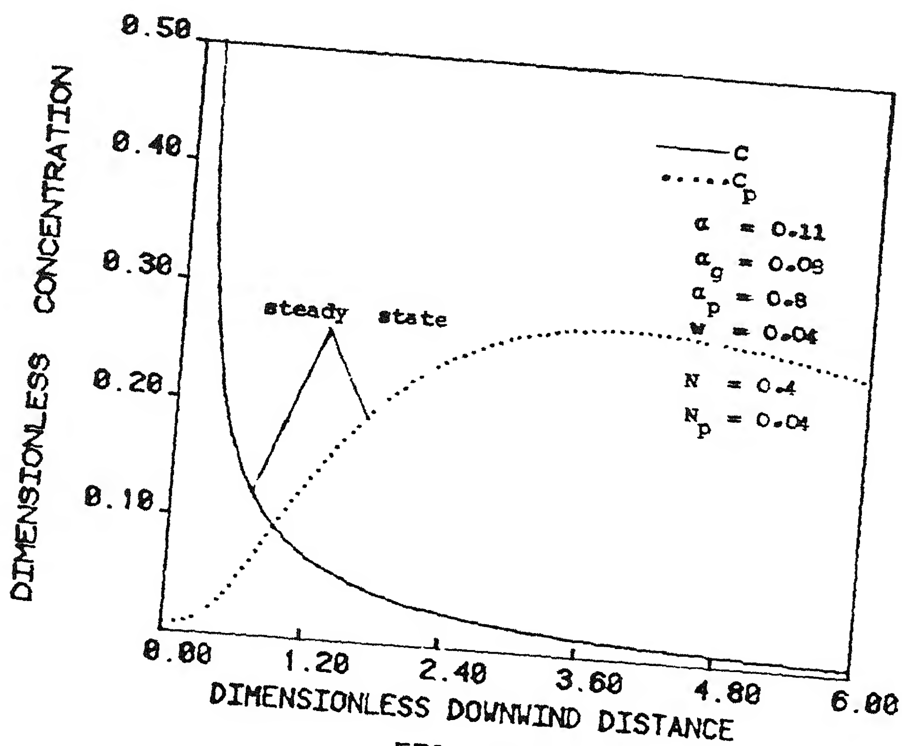


FIG 4.8

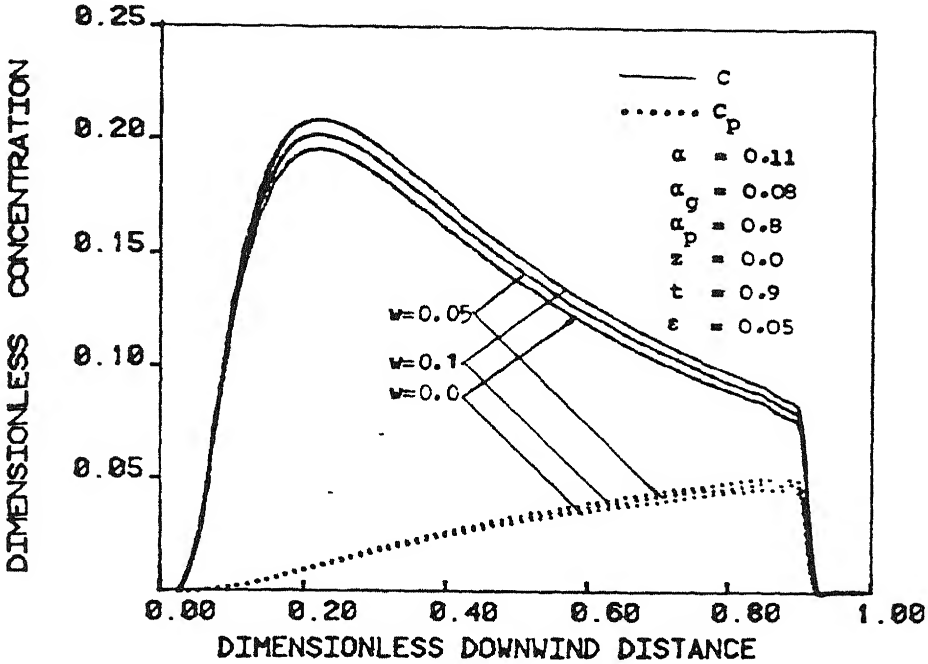


FIG 4.9 EFFECT OF SETTLING VELOCITY ON THE CONCENTRATION DISTRIBUTION.

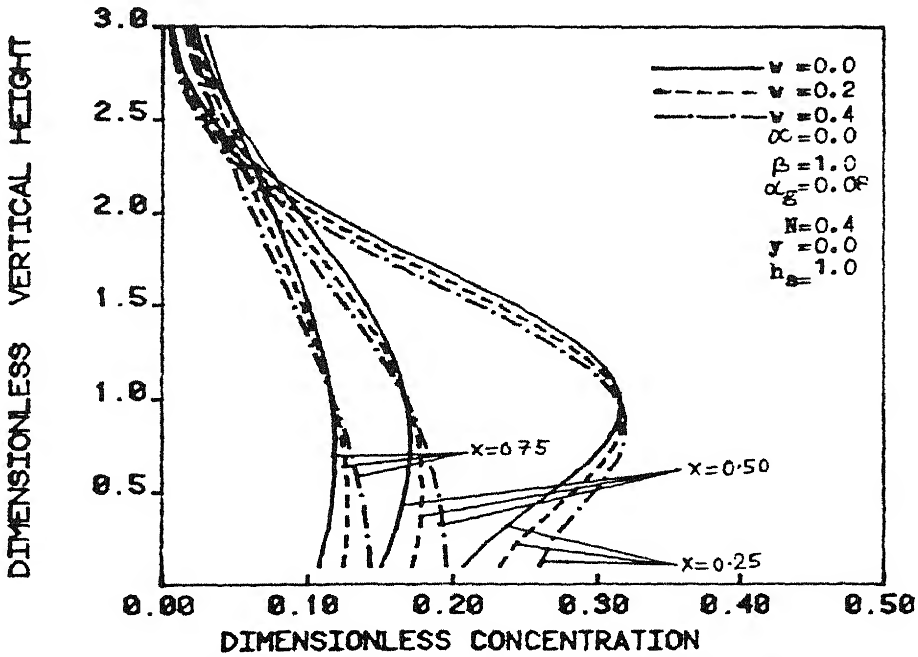


FIG4.10 CONCENTRATION PROFILE IN THE CASE OF POINT SOURCE

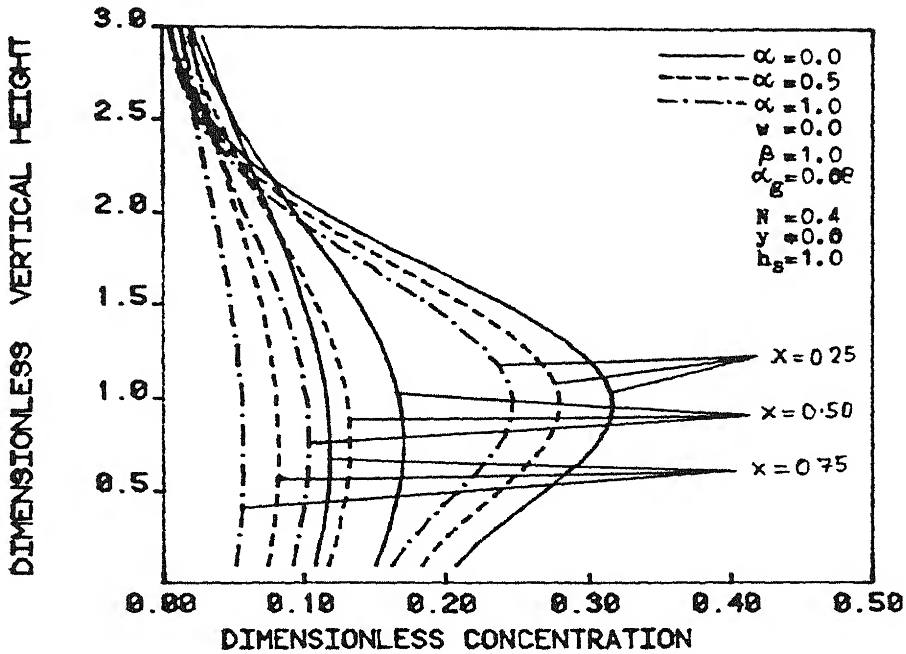


FIG 4.11 CONCENTRATION PROFILE IN THE CASE OF POINT SOURCE

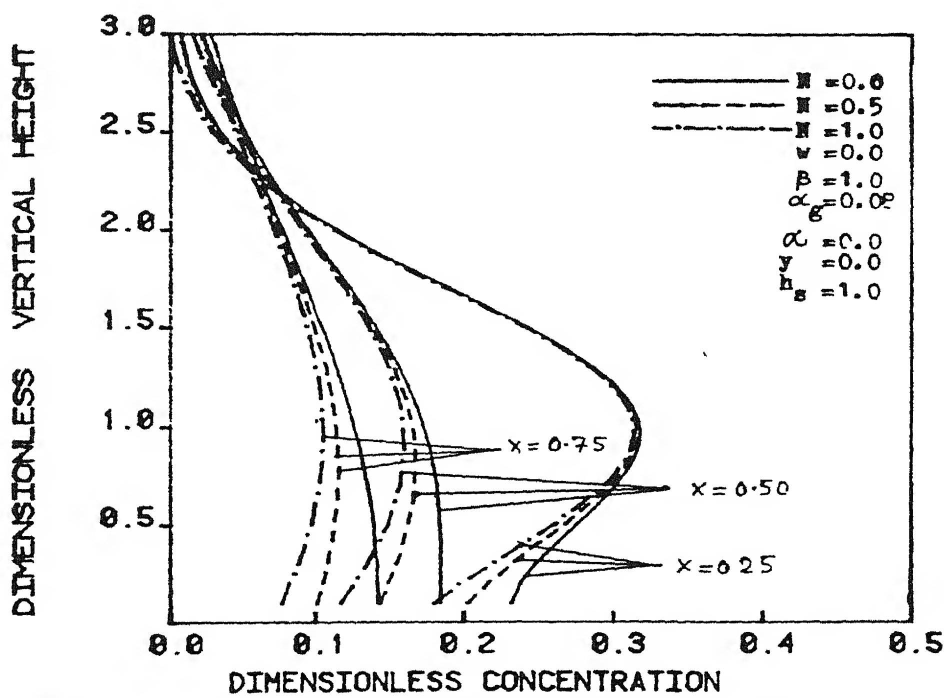


FIG 4.12 CONCENTRATION PROFILE IN THE CASE OF POINT SOURCE.

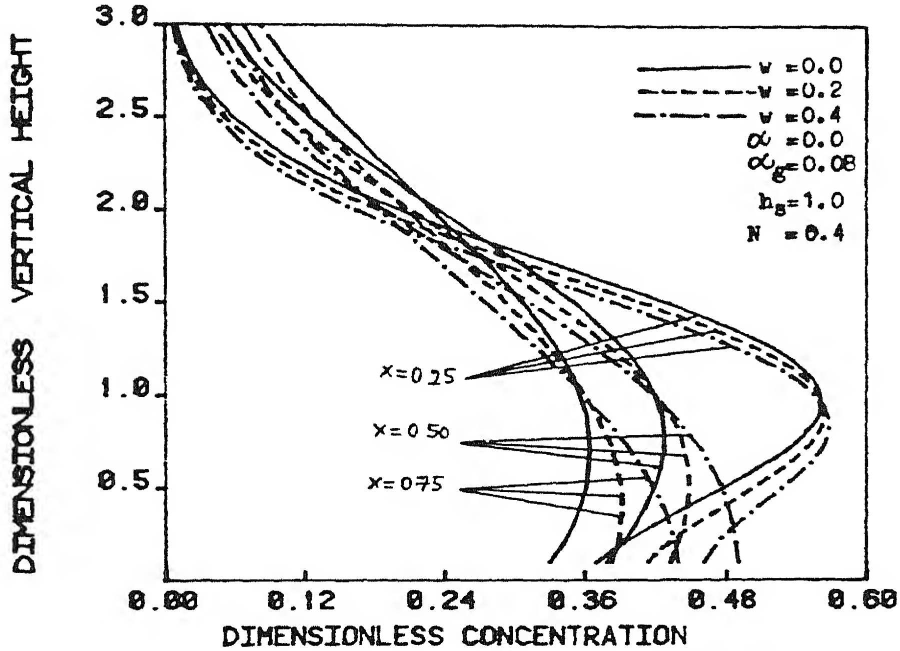


FIG 4.13 CONCENTRATION PROFILE IN THE CASE OF LINE SOURCE

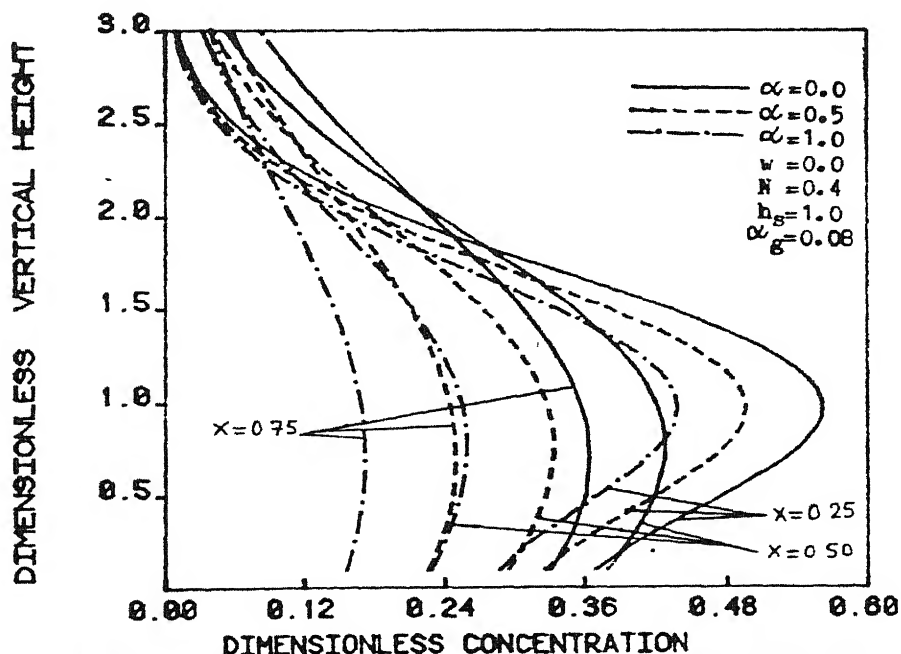


FIG4.14 CONCENTRATION PROFILE IN THE CASE OF LINE SOURCE

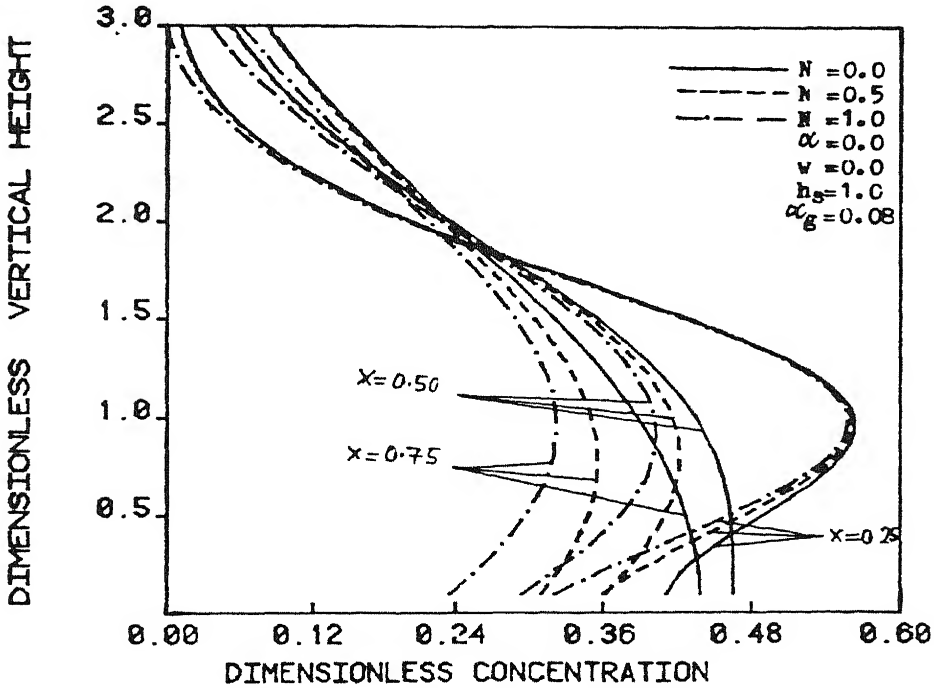


FIG 4.15 CONCENTRATION PROFILE IN THE CASE OF LINE SOURCE

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CHAPTER - V

DISPERSION OF A REACTIVE AIR POLLUTANT FROM A TIME DEPENDENT POINT SOURCE FORMING SECONDARY POLLUTANT: WITH INVERSION CONDITION

5.1 INTRODUCTION

In the previous chapter, effects of chemical reaction, settling velocity, dry and wet depositions on the unsteady state dispersion of a reactive air pollutant from a time dependent source have been discussed (without inversion condition). In this chapter the same problem is studied under the inversion condition. In this case, there exists a layer above the ground at height $z = H$ (say) which inhibits the vertical mixing of air pollutant. Mathematically this aspect can be represented by

$$J_z(x,y,z) = -K_z \frac{\partial C}{\partial z} - wc = 0 \text{ at } z = H$$

where J_z is flux in the z-direction, K_z is diffusion coefficient in z-direction, w is settling velocity of the pollutant.

As in the previous chapter, the following forms of flux are prescribed at the source to study the concentration distributions of both primary and secondary pollutants :

(i) instantaneous source,

(ii) constant source,

(iii) step function type source.

The case (iii) has also been applied to study the leakage of MIC gas in Bhopal, India.

5.2 MATHEMATICAL FORMULATION

Consider the dispersion of a reactive air pollutant in presence of an inversion layer from a time dependent point source located at height h_s above the ground and forming a secondary pollutant. The unsteady state diffusion equation governing the concentration C of primary pollutant can be written as follows,

$$\frac{\partial C}{\partial t} + U\frac{\partial C}{\partial x} - w\frac{\partial C}{\partial z} = K_y\frac{\partial^2 C}{\partial y^2} + K_z\frac{\partial^2 C}{\partial z^2} - (k+k_g)C \tag{5.1}$$

where the x-axis is along the wind direction, z-axis towards vertical height, U is wind velocity and K_y, K_z are diffusivity coefficients in y-, z-directions respectively. The constant k is the rate of conversion of C to secondary pollutant and k_g is its removal rate.

The initial and boundary conditions for C are

$$C(x,y,z,t) = 0 \quad \text{at } t = 0,\ x,y,z > 0 \tag{5.2}$$

$$C(x,y,z,t) = \frac{W(t)}{U}\,\delta(y)\,\delta(z-h_s) \quad \text{at } x = 0 \tag{5.3}$$

$$C(x,y,z,t) = 0 \quad \text{as } y \to \pm\infty \qquad t \geq 0 \tag{5.4}$$

$$K_z\frac{\partial C}{\partial z} + wC = v_d\,C \quad \text{at } z = 0 \qquad t \geq 0 \tag{5.5}$$

Assuming that there exists an inversion layer at height H which inhibits vertical mixing, we have

$$K_z \frac{\partial C}{\partial z} + wC = 0 \qquad \text{at } z = H \tag{5.6}$$

As in the previous chapter, the following forms of W(t) are considered in the subsequent analysis :

(i) Instantaneous source

$$W(t) = W_o\, \delta(t) \tag{5.7}$$

(ii) Constant source

$$W(t) = W_c \text{ (constant)}$$

(iii) Step function type source

$$W(t) = W_c \qquad 0 < t \leq t_o$$

$$= 0 \qquad t > t_o.$$

The atmospheric diffusion equation governing the concentration C_p of secondary pollutant can similarly be written as

$$\frac{\partial C_p}{\partial t} + U \frac{\partial C_p}{\partial x} - w \frac{\partial C_p}{\partial z} = K_y \frac{\partial^2 C_p}{\partial y^2} + K_z \frac{\partial^2 C_p}{\partial z^2} + kC - k_p C_p \tag{5.8}$$

where k_p is the rate of removal of C_p.

If there is no direct emission of secondary pollutant from the source the initial and boundary conditions for C_p can be considered as

$$C_p(x,y,z,t) = 0 \qquad \text{at } t = 0 \tag{5.9}$$

$$C_p(x,y,z,t) = 0 \qquad \text{at } x = 0 \tag{5.10}$$

$$C_p(x,y,z,t) = 0 \quad \text{as } y \to \pm\infty \tag{5.11}$$

$$K_z \frac{\partial C_p}{\partial z} + w\, C_p = v_{d_p}\, C_p \quad \text{at } z = 0 \tag{5.12}$$

$$K_z \frac{\partial C_p}{\partial z} + w\, C_p = 0 \quad \text{at } z = H \tag{5.13}$$

Using the following dimensionless variables

$$\bar{t} = \frac{K_z t}{H^2}\,,\ \bar{x} = \frac{K_z x}{UH^2}\,,\ \bar{y} = \frac{y}{H}\,,\ \bar{z} = \frac{z}{H}\,,$$

$$\bar{h}_s = \frac{h_s}{H}\,,\ \bar{C} = \frac{UH^2 C}{W}\,,\ \bar{C}_p = \frac{UH^2 C_p}{W}\,,\ \bar{w} = \frac{wH}{K_z}$$

$$\bar{W}(t) = \frac{W(t)}{W_c}\,,\ \bar{W}_o = \frac{W_o}{W_c}\frac{H^2}{K_z}\,. \tag{5.14}$$

equations (5.1 - 5.13) can be transformed in the dimensionless form as (dropping bars for convenience)

$$\frac{\partial C}{\partial t} + \frac{\partial C}{\partial x} - w\frac{\partial C}{\partial z} = \beta\frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2} - (\alpha+\alpha_g)C \tag{5.15}$$

$$C(x,y,z,t) = 0 \quad \text{at } t = 0 \tag{5.16}$$

$$C(x,y,z,t) = W(t)\,\delta(y)\,\delta(z-h_s) \quad \text{at } x = 0 \tag{5.17}$$

$$C(x,y,z,t) = 0 \quad \text{as } y \to \pm\infty \tag{5.18}$$

$$\frac{\partial C}{\partial z} + wC = NC \quad \text{at } z = 0 \tag{5.19}$$

$$\frac{\partial C}{\partial z} + wC = 0 \quad \text{at } z = 1 \tag{5.20}$$

$$\begin{aligned}
&\text{(i)} \quad W(t) = W_o\,\delta(t) \\
&\text{(ii)} \quad W(t) = 1 \\
&\text{(iii)} \quad W(t) = 1 \qquad 0 < t \le t_o \\
&\qquad\qquad\quad\ = 0 \qquad t > t_o
\end{aligned} \tag{5.21}$$

$$\frac{\partial C_p}{\partial t} + \frac{\partial C_p}{\partial x} - w\frac{\partial C_p}{\partial z} = \beta\frac{\partial^2 C_p}{\partial y^2} + \frac{\partial^2 C_p}{\partial z^2} + \alpha C - \alpha_p C_p \tag{5.22}$$

$$C_p(x,y,z,t) = 0 \quad \text{at } t = 0 \tag{5.23}$$

$$C_p(x,y,z,t) = 0 \quad \text{at } x = 0 \tag{5.24}$$

$$C_p(x,y,z,t) = 0 \quad \text{as } y \to \pm\infty \tag{5.25}$$

$$\frac{\partial C_p}{\partial z} + w\, C_p = N_p\, C_p \quad \text{at } z = 0 \tag{5.26}$$

$$\frac{\partial C_p}{\partial z} + w\, C_p = 0 \quad \text{at } z = 1 \tag{5.27}$$

where $\beta = \dfrac{K_y}{K_z}$, $\alpha = \dfrac{kH^2}{K_z}$, $\alpha_g = \dfrac{k_g H^2}{K_z}$, $N = \dfrac{v_d H}{K_z}$

$\alpha_p = \dfrac{k_p H^2}{K_z}$, $N_p = \dfrac{v_{d_p} H}{K_z}$.

5.3 METHOD OF SOLUTION

As in Chapter II, following Astarita et al. (1979), Alam and Seinfeld (1981), equations (5.15) and (5.22) can be written as uncoupled system :

$$LC - (\alpha + \alpha_g)C = 0 \tag{5.28}$$

$$LB - \alpha_p B = 0 \tag{5.29}$$

where

$$L = -\frac{\partial}{\partial t} - \frac{\partial}{\partial x} + w\frac{\partial}{\partial z} + \beta\frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

$$B = C_p(x,y,z,t) - \frac{\alpha C(x,y,z,t)}{(\alpha_p - \alpha - \alpha_g)}. \tag{5.30}$$

The boundary conditions for B are

$$B(x,y,z,t) = 0 \qquad \text{at } t = 0 \tag{5.31}$$

$$B(x,y,z,t) = \frac{-\alpha}{\alpha_p - \alpha - \alpha_g} W(t)\, \delta(y)\, \delta(z-h_s) \text{ at } x = 0 \tag{5.32}$$

$$B(x,y,z,t) = 0 \quad \text{as } y \to \pm\infty \tag{5.33}$$

$$\frac{\partial B}{\partial z} = (N_p - w)B + \frac{\alpha(N_p - N)C}{(\alpha_p - \alpha - \alpha_g)} \text{ at } z = 0 \tag{5.34}$$

$$\frac{\partial B}{\partial z} + wB = 0 \qquad \text{at } z = 1. \tag{5.35}$$

Introducing the transformations

$$C = C_1\, e^{-\frac{w}{2}(z-h_s) - \frac{w^2}{4} x} \tag{5.36}$$

$$B = B_1\, e^{-\frac{w}{2}(z-h_s) - \frac{w^2}{4} x}$$

we have from equations (5.28 - 5.35)

$$\frac{\partial C_1}{\partial t} + \frac{\partial C_1}{\partial x} = \beta \frac{\partial^2 C_1}{\partial y^2} + \frac{\partial^2 C_1}{\partial z^2} - (\alpha + \alpha_g) C_1 \tag{5.37}$$

$$\frac{\partial B_1}{\partial t} + \frac{\partial B_1}{\partial x} = \beta \frac{\partial^2 B_1}{\partial y^2} + \frac{\partial^2 B_1}{\partial z^2} - \alpha_p B_1 \tag{5.38}$$

and boundary conditions are

$$C_1 = 0 \quad \text{as } y \to \pm\infty, \quad \text{at } t = 0 \tag{5.39}$$

$$B_1 = 0 \quad \text{as } y \to \pm\infty, \text{ at } t = 0 \tag{5.40}$$

$$C_1 = W(t)\,\delta(y)\,\delta(z-h_s)\quad e^{\frac{W}{2}(z-h_s)} \quad \text{at } x = 0 \tag{5.41}$$

$$B_1 = \frac{-\alpha}{\alpha_p-\alpha-\alpha_p}\,W(t)\,\delta(y)\,\delta(z-h_s)\quad e^{\frac{W}{2}(z-h_s)} \quad \text{at } x = 0 \tag{5.42}$$

$$\frac{\partial C_1}{\partial z} = (N - \frac{W}{2})C_1 \quad \text{at } z = 0 \tag{5.43}$$

$$\frac{\partial C_1}{\partial z} + \frac{W}{2}\,C_1 = 0 \quad \text{at } z = 1 \tag{5.44}$$

$$\frac{\partial B_1}{\partial z} = (N_p - \frac{W}{2})B_1 + \frac{\alpha(N_p-N)}{\alpha_p-\alpha-\alpha_g}\,C_1 \quad \text{at } z = 0 \tag{5.45}$$

$$\frac{\partial B_1}{\partial z} + \frac{W}{2}\,B_1 = 0 \quad \text{at } z = 1. \tag{5.46}$$

The solutions for both C_1 and B_1 are obtained by using Laplace, Fourier transforms and method of separation of variables. We have

$$C_1 = W_o\,P^*(x,y,z)\,\delta(t-x) \tag{5.47}$$

$$B_1 = W_o\,Q^*(x,y,z)\,\delta(t-x) \tag{5.48}$$

where,

$$P^*(x,y,z) = \frac{\exp(-y^2/4\beta x)}{\sqrt{4\pi\beta x}}\,\exp(-(\alpha+\alpha_g)x).$$

$$\times \sum_{n=1}^{\infty} \frac{2(\lambda_n^2 + \frac{W^2}{4})(\lambda_n \cos\lambda_n h_s + N_1 \sin\lambda_n h_s) \times (\lambda_n \cos\lambda_n z + N_1 \sin\lambda_n z)}{(\lambda_n^2+N_1^2)(\lambda_n^2 + \frac{W^2}{4} + \frac{W}{2}) + N_1(\lambda_n^2 + \frac{W^2}{4})}\; e^{-\lambda_n^2 x}$$

$$Q^*(x,y,z) = \frac{\exp(-y^2/4\beta x)}{\sqrt{4\pi\beta x}} \frac{\alpha}{(\alpha_p-\alpha-\alpha_g)}$$

$$\times \sum_{n=1}^{\infty} \frac{2(\mu_n + \frac{w^2}{4})(\mu_n \cos\mu_n z + N_{p1} \sin\mu_n z)}{\{(\mu_n^2 + \frac{w^2}{4} + \frac{w}{2})(\mu_n^2 + N_{p1}^2) + N_{p1}(\mu_n^2 + \frac{w^2}{4})\}} e^{-(\alpha_p + \mu_n^2)x}$$

$$\times \{\frac{(N - N_p)(2+w(1-z))}{(w + N_{p1}(2+w))} (\mu_n \sin\mu_n + N_{p1}(1-\cos\mu_n))$$

$$\times \sum_{m=1}^{\infty} \frac{2(\lambda_m^2 + \frac{w^2}{4})\lambda_m(\lambda_m \cos\lambda_m h_s + N_1 \sin\lambda_m h_s)}{(\lambda_m^2+N_1^2)(\lambda_m^2 + \frac{w^2}{4} + \frac{w}{2}) + N_1(\lambda_m^2 + \frac{w^2}{4})} \int_0^x e^{-(\alpha+\alpha_g-\alpha_p-\mu_n^2+\lambda_m^2)x'} dx'$$

$$- (\mu_n \cos\mu_n h_s + N_{p1} \sin\mu_n h_s)\}$$

$$N_1 = N - \frac{w}{2}$$

$$N_{p1} = N_p - \frac{w}{2}$$

and λ_n's, μ_n's are roots of following transcedental equations,

$$\tan\lambda_n = \frac{\lambda_n(N_1 + \frac{w}{2})}{(\lambda_n^2 - \frac{w}{2} N_1)}$$

$$\tan\mu_n = \frac{\mu_n(N_{p1} + \frac{w}{2})}{(\mu_n^2 - \frac{w}{2} N_{p1})}$$

and $\delta(t-x)$ is Dirac-delta function.

(ii) For constant source

$$C_1 = P^*(x,y,z)\, H(t-x) \tag{5.49}$$

$$B_1 = Q^*(x,y,z)\ H(t-x). \tag{5.50}$$

It is observed from above equations that C_1 and B_1 are independent of time as $t \to \infty$. This implies that both concentrations C and C_p reach to steady state.

(iii) For step function type source

$$C_1 = P^*(x,y,z)\ [H(t-x)-H(t-t_o-x)\ H(t-t_o)] \tag{5.51}$$

$$B_1 = Q^*(x,y,z)\ [H(t-x)-H(t-t_o-x)\ H(t-t_o)] \tag{5.52}$$

Finally the solutions for C and B in each case can be obtained as follows :

(i) For instantaneous source

$$C(x,y,z,t)=W_oP^*(x,y,z)\delta(t-x)\exp\{-\frac{w}{2}(z-h_s)-\frac{w^2}{4}x\} \tag{5.53}$$

$$B(x,y,z,t)=W_oQ^*(x,y,z)\delta(t-x)\exp\{-\frac{w}{2}(z-h_s)-\frac{w^2}{4}x\} \tag{5.54}$$

(ii) For the constant source

$$C(x,y,z,t) = P^*(x,y,z)\ H(t-x)\exp\{-\frac{w}{2}\ (z-h_s) - \frac{w^2}{4}x\} \tag{5.55}$$

$$B(x,y,z,t) = Q^*(x,y,z)\ H(t-x)\exp\{-\frac{w}{2}\ (z-h_s) - \frac{w^2}{4}x\}. \tag{5.56}$$

It is noted here that as $t \to \infty$ and $w = 0$ the above equations reduce to the same form as obtained by Alam and Seinfeld (1981).

(iii) For step function type source

$$C(x,y,z,t) = P^*(x,y,z)\ [H(t-x)-H(t-t_o-x)\ H(t-t_o)] \times$$
$$\times \exp\{-\frac{w}{2}(z-h_s) - \frac{w^2}{4}x\} \qquad (5.57)$$

$$B(x,y,z,t) = Q^*(x,y,z)\ [H(t-x)-H(t-t_o-x)\ H(t-t_o)] \times$$
$$\times \exp\{-\frac{w}{2}(z-h_s) - \frac{w^2}{4}x\}. \qquad (5.58)$$

5.4 SOLUTIONS FOR THE LINE SOURCE

The solutions are obtained for the line source by integrating equations (5.53 - 5.58) with respect to y between $-\infty$ to ∞ and are written in each case as follows :

(i) For instantaneous source

$$C(x,z,t) = W_o\ P^*(x,z)\ \delta(t-x) \qquad (5.59)$$

$$C_p(x,z,t) = W_o\ Q^*(x,z)\ \delta\ (t-x) + \frac{\alpha C(x,z,t)}{(\alpha_p-\alpha-\alpha_g)} \qquad (5.60)$$

where

$$P^*(x,z) = \exp\{-(\alpha+\alpha_g + \frac{w^2}{4})x - \frac{w}{2}(z-h_s)\}$$

$$\times \sum_{n=1}^{\infty} \frac{2(\lambda_n^2 + \frac{w^2}{4})(\lambda_n \cos\lambda_n h_s + N_1 \sin\lambda_n h_s)}{\{(\lambda_n^2+N_1^2)(\lambda_n^2 + \frac{w^2}{4} + \frac{w}{2}) + N_1(\lambda_n^2 + \frac{w^2}{4})\}} \times$$

$$(\lambda_n \cos\lambda_n z + N_1 \sin\lambda_n z)\ e^{-\lambda_n^2 x}$$

$$Q^*(x,z) = \frac{\alpha}{\alpha_p-\alpha-\alpha_g} \sum_{n=1}^{\infty} \frac{(\mu_n^2 + \frac{w^2}{4})(\mu_n \cos\mu_n z+N_{p1} \sin\mu_n z)}{\{(\mu_n^2 + \frac{w^2}{4} + \frac{w}{2})(\mu_n^2+N_{p1}^2)+N_{p1}(\mu_n^2 + \frac{w^2}{4})\}} \times$$

$$\exp(-(\alpha_p+\mu_n^2)x)\{\frac{(N-N_p)(2+w(1-z))}{(w+N_{p1}\ (2+w))}\ (\mu_n \sin\mu_n+N_{p1}(1-\cos\mu_n))$$

$$\times \sum_{m=1}^{\infty} \frac{2(\lambda_m^2 + \frac{w^2}{4})\ \lambda_m(\lambda_m \cos\lambda_m h_s + N_1 \sin\lambda_m h_s)}{\{(\lambda_m^2+N_1^2)(\lambda_m^2 + \frac{w^2}{4} + \frac{w}{2}) + N_1(\lambda_m^2 + \frac{w^2}{4})\}}$$

$$\times \int_0^x \exp\left[-(\alpha+\alpha_g-\alpha_p-\mu_n^2 + \lambda_m^2)x'\right] dx' - (\mu_n \cos\mu_n h_s + N_{p1} \sin\mu_n h_s)\}$$

(ii) For constant source

$$C(x,z,t) = P^*(x,z)\ H(t-x) \tag{5.61}$$

$$C_p(x,z,t) = Q^*(x,z)\ H(t-x) + \frac{\alpha\ C(x,z,t)}{(\alpha_p-\alpha-\alpha_g)} \tag{5.62}$$

(iii) For step function type source

$$C(x,z,t) = P^*(x,z)\ [H(t-x)-H(t-t_o-x)\ H(t-t_o)]$$

$$C_p(x,z,t) = Q^*(x,z)\ [H(t-x)-H(t-t_o-x)\ H(t-t_o)] + \frac{\alpha\ C(x,z,t)}{(\alpha_p - \alpha - \alpha_g} .$$

5.5 RESULTS AND DISCUSSION

The effects of various parameters on the central line $(0,0,h_s)$ concentrationsof both species in all the three cases are depicted in figs. (5.1 - 5.7) for different values of t, $\beta = 10.0$, $N = 2.0$, $N_p = 0.2$, $w = 0.2$, $y = 0.0$, $h_s = 0.2$. It is noted that the concentration C decreases as α increases but C_p increases in all cases at a particular time and location (see fig. 5.7 for example in the case of constant source strength). It is also seen that the concentrationsof both the species decrease as downwind distance increases. The effect of removal is to decrease the concentrations of both species.

When the source strength is instantaneous the central line concentration distributions are shown in figs. (5.1 - 5.2) for different values of t, $W_o = 1.0$, $\alpha = 2.77$, $\alpha_g = 0.0, 2.0$ and $\alpha_p = 0.0, 20.0$. It is seen that C and C_p decrease as time increases, the concentration C_p being less than C for the set of parameters chosen in graphs(5.1 - 5.2).

When the source strength is constant, the central line concentrations of both the species are plotted in figs. (5.3 - 5.4) for different values of t, $\alpha = 2.77$, $\alpha_g = 0.0, 2.0$ and $\alpha_p = 0.0, 20.0$, $W = 0.2$. From these figures, it is found that the concentrations of both the species C, C_p are zero for $t < x$. It implies that the pollutant front has not reached the point x as yet. The concentrations C and C_p increase as time increases and reach to their respective steady state values as $t \to \infty$.

When the flux is given by the step-function type, the central line concentrations C and C_p decrease as time increases for $t > t_o$ (see fig. 5.5 - 5.6) and for $t \leq t_o$, the behaviour is similar as in the case of constant flux.

The effect of settling velocity on the unsteady state ground level concentration is also studied and it is found that the concentration of primary species increases as settling velocity increases (see fig. 5.8 for the case of constant flux).

In the case of line source, similar results have been found in all the three cases (graphs are not depicted).

The effect of settling velocity, chemical reaction and dry deposition on the vertical concentration distributions of primary species in the case of constant flux for both point and line sources are depicted in figs. (5.9 - 5.14). It is seen from figs. (5.9, 5.12) that as settling velocity increases the concentration C increases below the source height, but reverse is the case above the source height. The effect of chemical reaction is to decrease the concentration of pollutants in the case of both point and line sources (see figs. 5.10, 5.13). The effect of ground level deposition parameter is shown in figs. (5.11, 5.14). It is observed that as deposition at the ground level increases the concentration decreases and this effect is more predominant below the source height.

5.6 EFFECT OF INVERSION LAYER ON THE DISPERSION OF POLLUTANT

To see the effect of inversion layer on the dispersion of a pollutant, we compare the corresponding concentration distributions in the case of a continuous point source as obtained in Chapter IV (without inversion condition) and in Chapter V (with inversion condition). The concentration of primary pollutant in dimensionless form (the dimensionless quantities is defined in Chapter IV, here h_a is taken source height h_s) is given as follows in the absence of inversion,

$$C(x,y,z) = \frac{\exp(-y^2/4\beta x)}{4\pi x\sqrt{\beta}}\, e^{-\frac{W}{2}(z-1)-(\frac{W^2}{4}+\alpha+\alpha_g)x}$$

$$\times \{ [e^{\frac{-(z-1)^2}{4x}} + e^{\frac{-(z+1)^2}{4x}}] - (4\pi x)^{1/2}\ (N - \tfrac{W}{2}) \times$$

5.7 APPLICATION OF CASE III : MIC LEAKAGE IN BHOPAL, INDIA

The dispersion of Methyl isocynate (MIC) leakage from Union Carbide Factory in Bhopal took place on Dec. 3, 1984 in the middle of night. It has been reported that at the time of episode a light breeze (12 km/hr) was blowing in south-south easterly direction which changed its direction towards south south-west and slowed down later. The temperature was around 12-14°C at that night. The MIC gas (approximately 40 tons) escaped through the nozzle of the 33 meter high ventline and leaked for about one hour (A report, 1984). This gas, being heavier than air, settled down over considerable areas of the city when the wind died down. The limit of region where people got seriously affected was about 8-9 Kms from the factory. The report also suggested that the gas travelled over 15 kilometers covering area of over 50 square Kms, affecting nearly two lakh people, constituting one fourth of the city population.

MIC is strongly toxic and highly unstable. It decomposes easily in the presence of moisture forming methyl amine according to following reaction

$$CH_3NCO + H_2O \rightarrow CH_3N = C\begin{matrix} OH \\ OH \end{matrix} \rightarrow CH_3NH_2 + CO_2$$

(MIC) (Methyl amine)

MIC affects all living beings including vegetation. In a report, it has been recorded that when four persons were exposed for 1 to 5 minutes, the following types of effect were noticed :

0.4 ppm	-	no effects
2.0 ppm	-	lachrymation, irritation in nose and throat
4.0 ppm	-	Symptoms of irritation more marked
21.0 ppm	-	Unbearable irritation of eyes,nose and throat.

In cases of prolonged exposure MIC acts by destroying protiens and lipids in the lungs. This leads to changes in the permeability of the lung membranes which get filled up with water causing death. The maximum permissible exposure limit for industrial workers prescribed is only one-fifth of one ppm for MIC.

The complete set of data is not available for MIC dispersion at the time of episode; the following parameters are, therefore, chosen in the computational analysis of Case (iii) being applied to Bhopal gas leakage (see Table 1) (A report, 1984).

Table 1

Parameters	Values of parameters chosen for MIC dispersion in the analysis	Non-dimensional Values
k	$0.05\ hr^{-1}$ (corresponding to SO_2)	$\alpha = 2.77$
k_g	0.0	$\alpha_g = 0.0$
k_p	0.0	$\alpha_p = 0.0$
v_d	2 cm/sec	$N = 4.0$
K_z	$5\ m^2/sec$	
$\frac{K_Y}{K_z} = \beta$	10.0	$\beta = 10$
U	12 Km/hr	
h_s	40 meter (effective height)	$h_s = 0.04$
t_o	One hour	$t_o = 0.018$
W	11.1 Kg/sec	
ε	6 minutes (approximately)	$\varepsilon = .002$
C	2 ppm	$C = 1.4537$
x	6.666 Km	$x = 0.01$

Using data in Table 1, the expression for C given by equation (5.57) is calculated for different values of $w = 0.0, 4.0$ by choosing the effective height of the source as 40 meters. As pointed out earlier, the leakage time t_o is taken as one hour (i.e. dimensionless $t_o = 0.018$).

The concentration distribution at $t = 0.018$ (one hour) for different values of $w = 0.0$, 4.0 are shown in fig. 5.17. It is seen from this graph that 2 ppm concentration line (dimensionless concentration $C = 1.4537$) intersects the concentration profile for $w = 0.0$ at a point which corresponds to a dimensionless distance 0.0163. This is equivalent to about 10.5 Kms. in the downwind direction. Also the 2 ppm concentration line intersects the concentration profile for $w = 4.0$ at the dimensionless distance 0.0172, which is equivalent to 11.5 kilometers. Similarly the concentration distributions at $t = 0.027$ ($1\frac{1}{2}$ hour) for different $w = 0.0$, $w = 4.0$ are depicted in fig. 5.18. It is also observed from these graphs (5.17-5.18) that as settling velocity increases the ground level concentration increases.

Since the limit for actual affected zone along the wind direction in the city (wind changed its direction during the episode) varied from 8-9 Kms. at different locations, the present analysis though approximate (wind velocity and diffusivities are assumed constant, change of wind direction ignored) provides useful information regarding the impact assessment of the dispersion of MIC leakage in Bhopal, India.

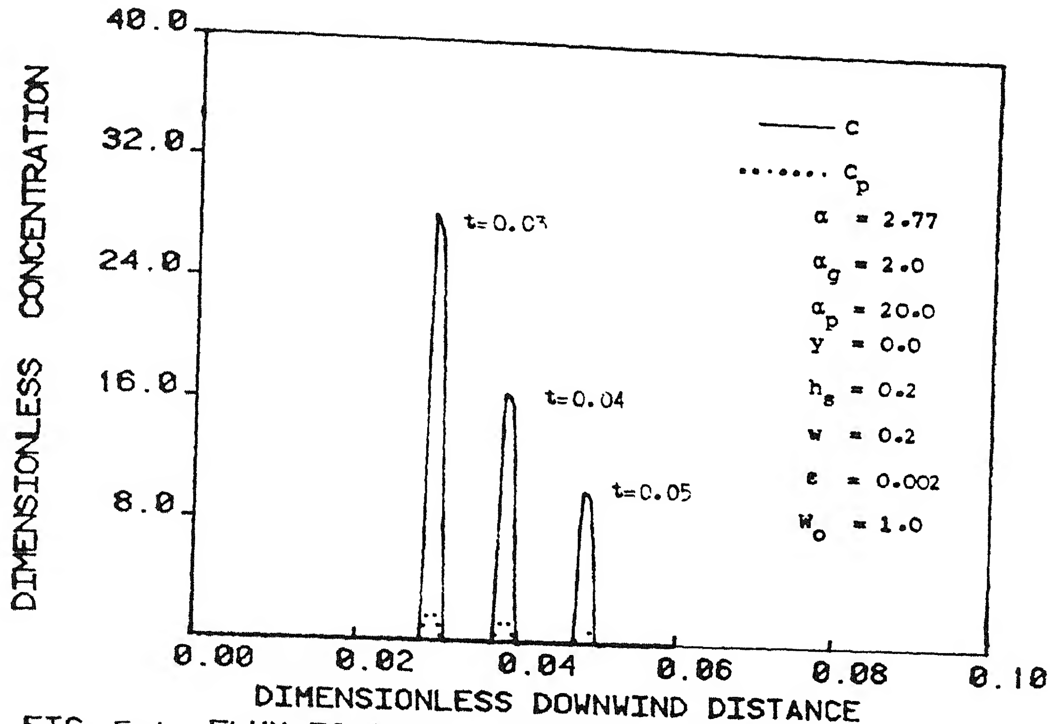

FIG 5.1 FLUX IS INSTANTANEOUS AT THE SOURCE

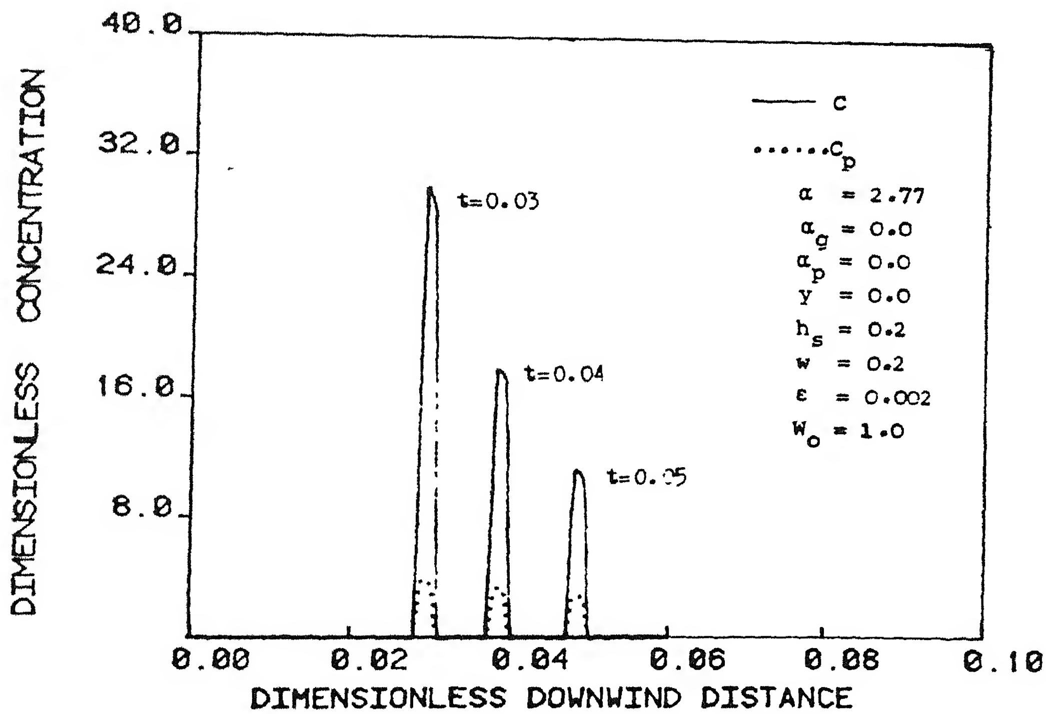

FIG 5.2 FLUX IS INSTANTANEOUS AT THE SOURCE.

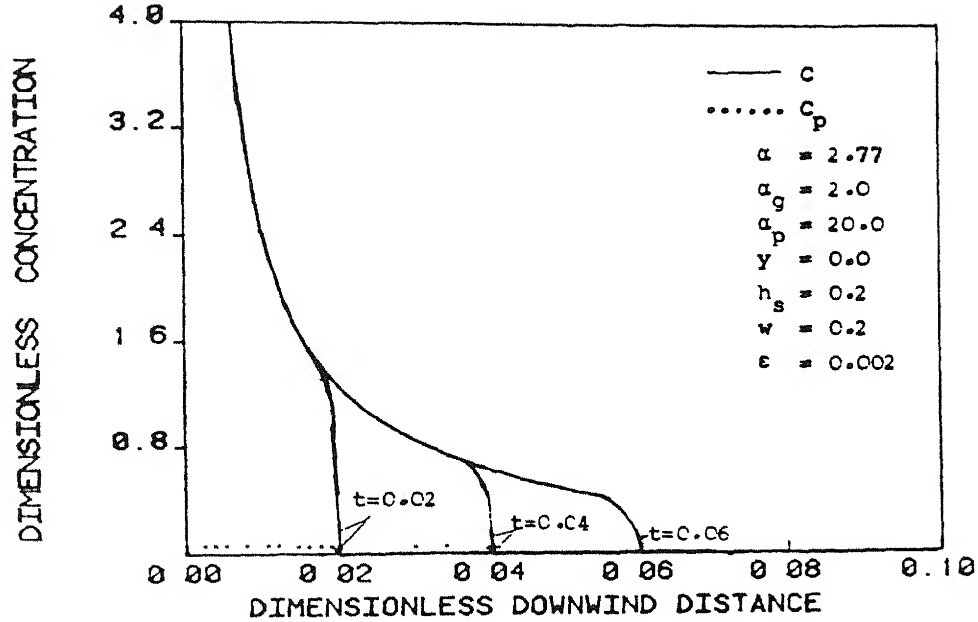

FIG 5 3 FLUX IS CONSTANT AT THE SOURCE

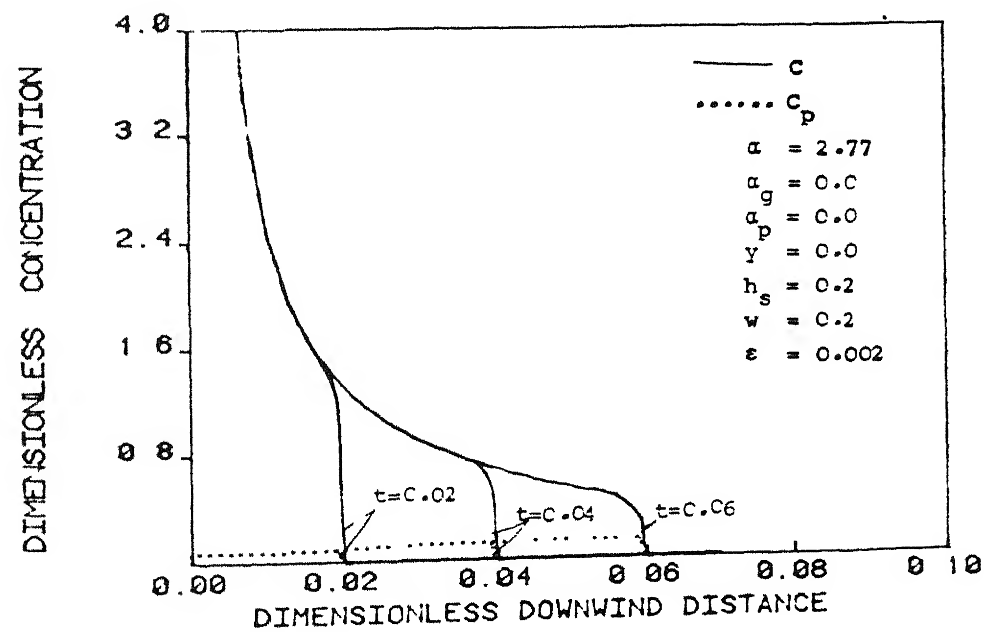

FIG 5.4 FLUX IS CONSTANT AT THE SOURCE

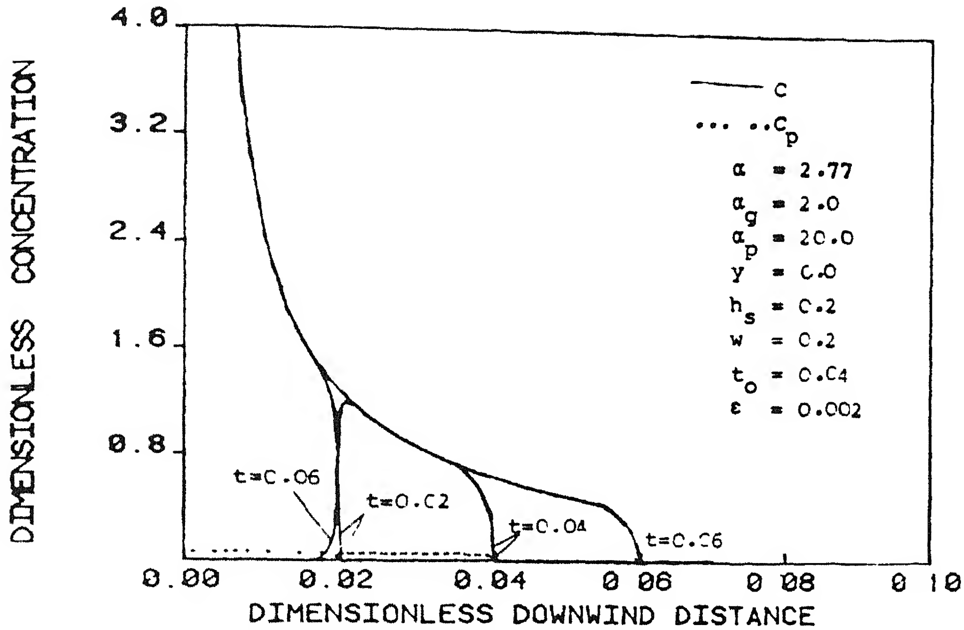

FIG 5 5 FLUX IS STEP FUNCTION TYPE AT THE SOURCE

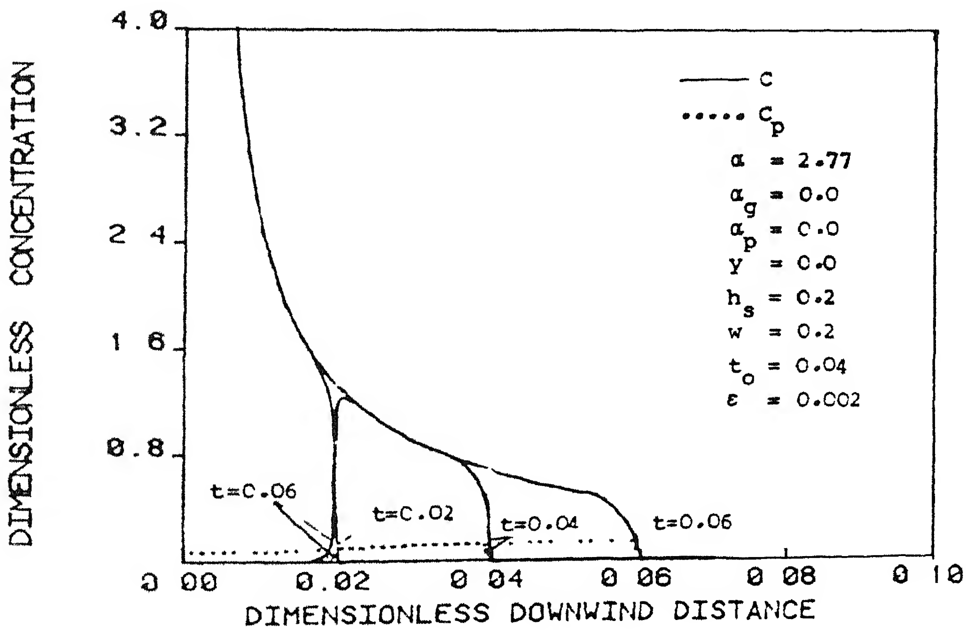

FIG 5 6 FLUX IS STEP FUNCTION TYPE AT THE SOURCE

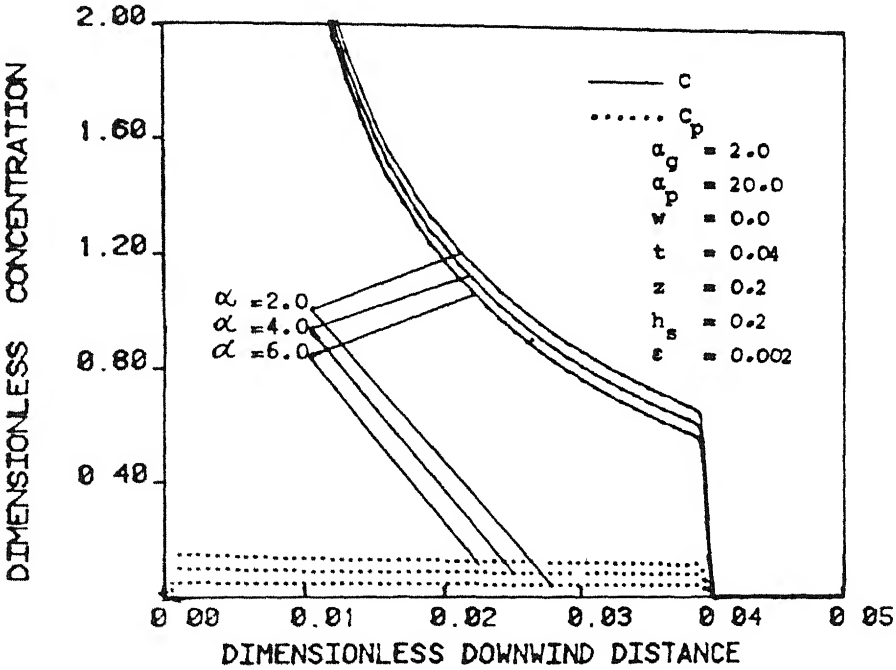

FIG 5 7 FLUX IS CONSTANT AT THE SOURCE

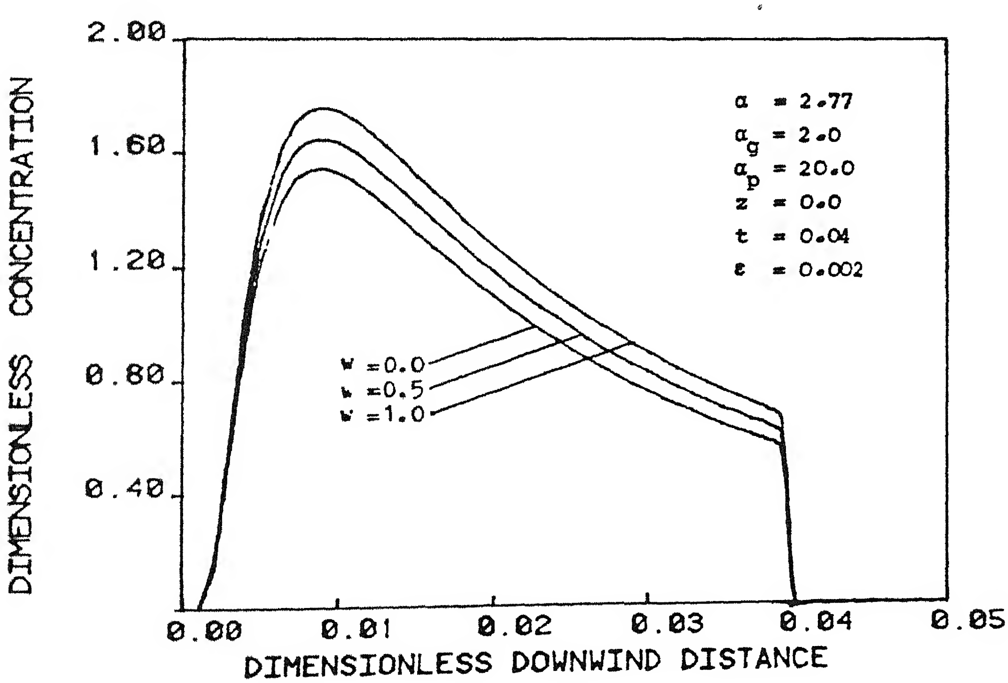

FIG5.8 EFFECT OF EETTLING VELOCITY ON THE GROUND LEVEL CONCENTRATION

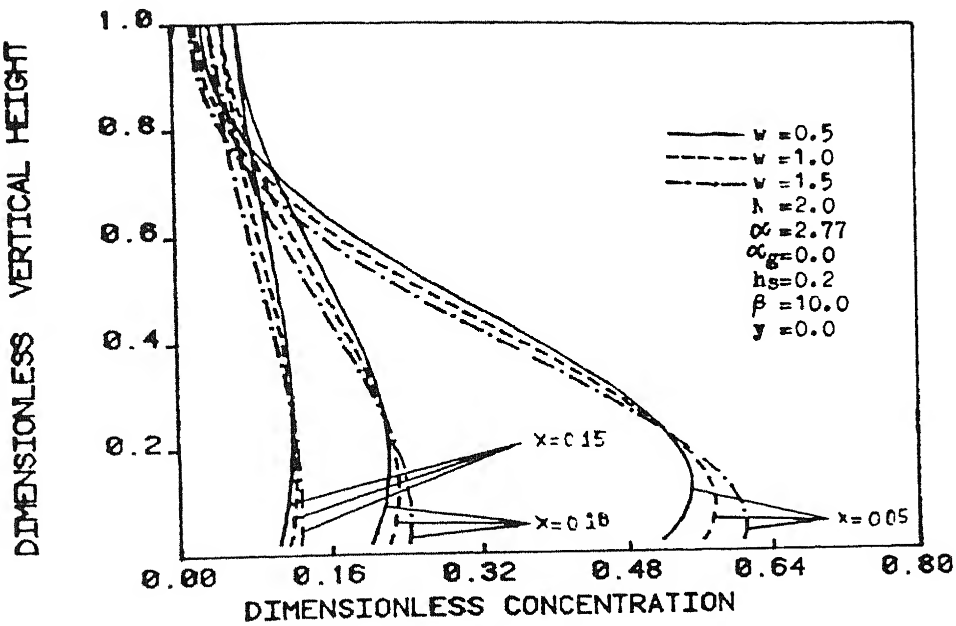

FIG 5.9 CONCENTRATION PROFILE IN THE CASE OF POINT SOURCE

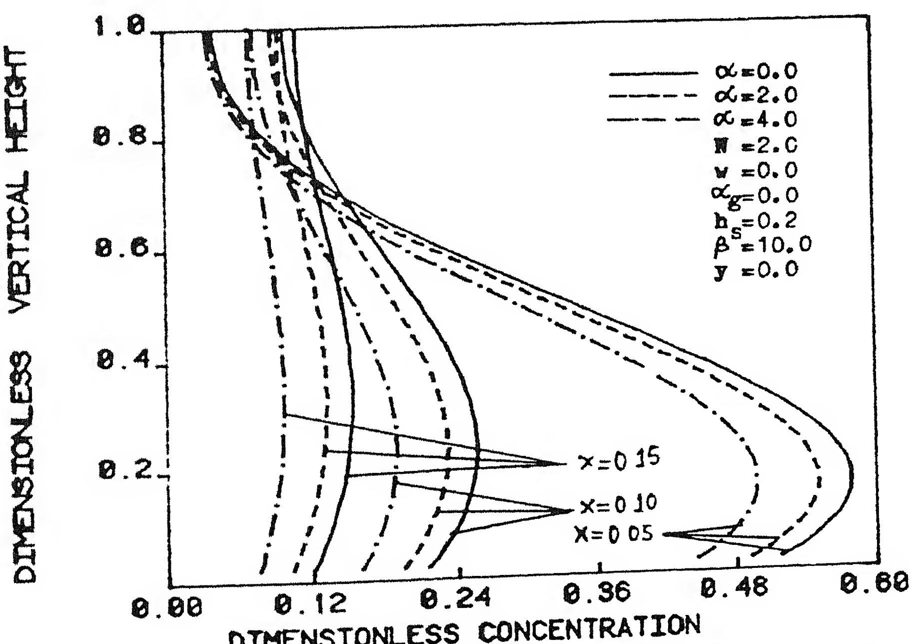

FIG 5.10 CONCENTRATION PROFILE IN THE CASE OF POINT SORUCE

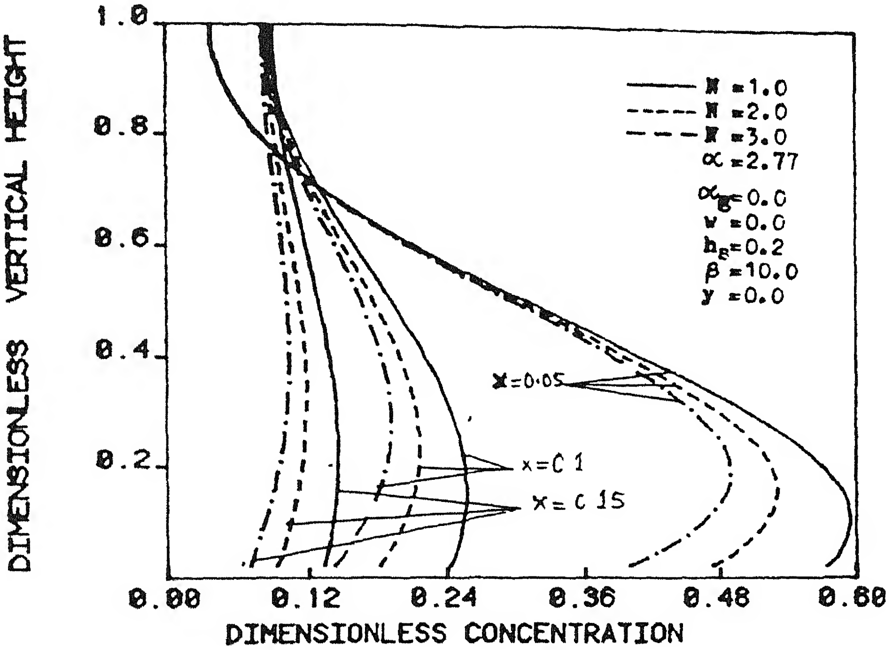

FIG 5.11 CONCENTRATION PROFILE IN THE CASE OF POINT SOURCE

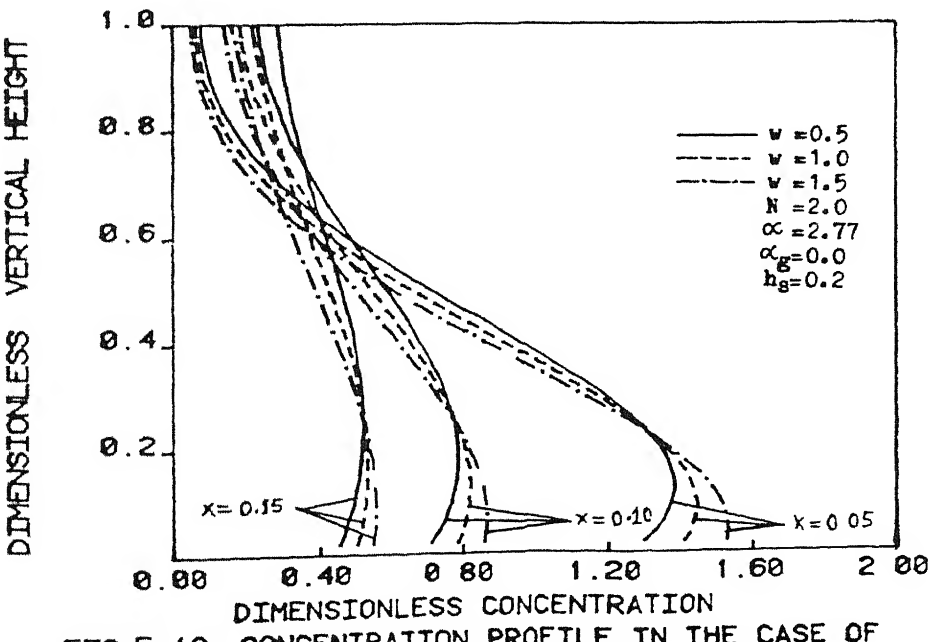

FIG 5.12 CONCENTRATION PROFILE IN THE CASE OF LINE SOURCE

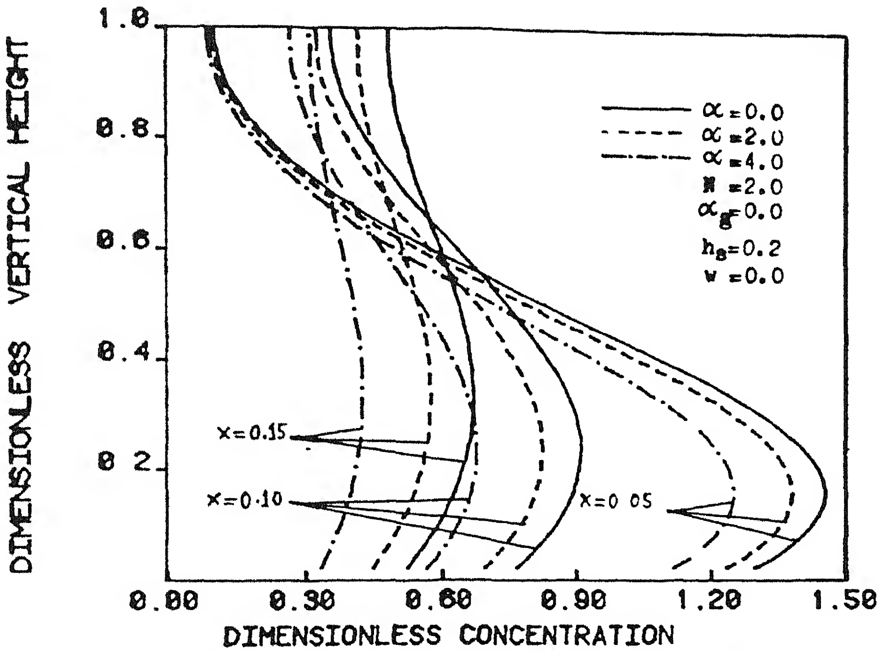

FIG 5.13 CONCENTRATION PROFILE IN THE CASE OF LINE SOURCE.

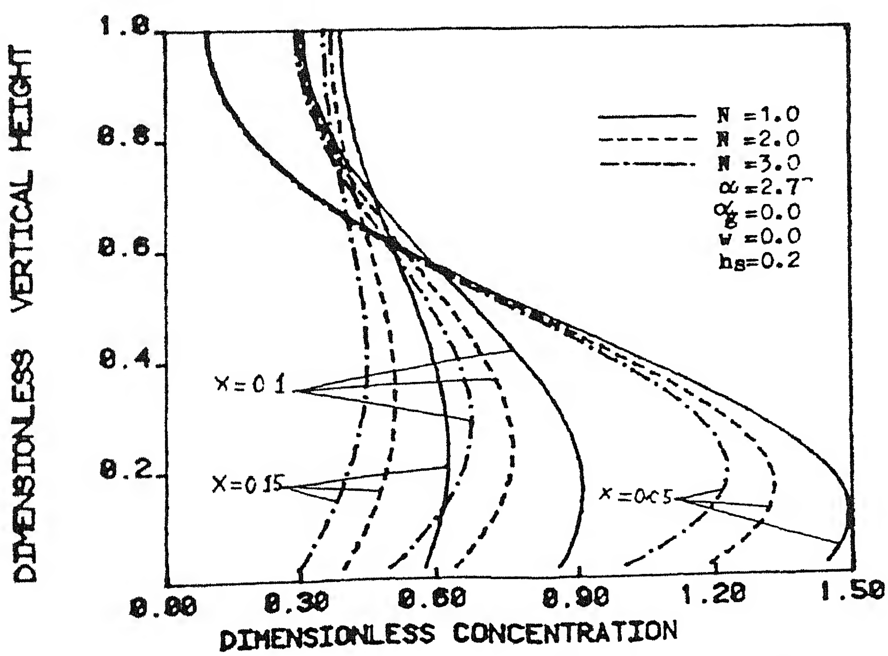

FIG 5.14 CONCENTRATION PROFILE IN THE CASE OF LINE SOURCE

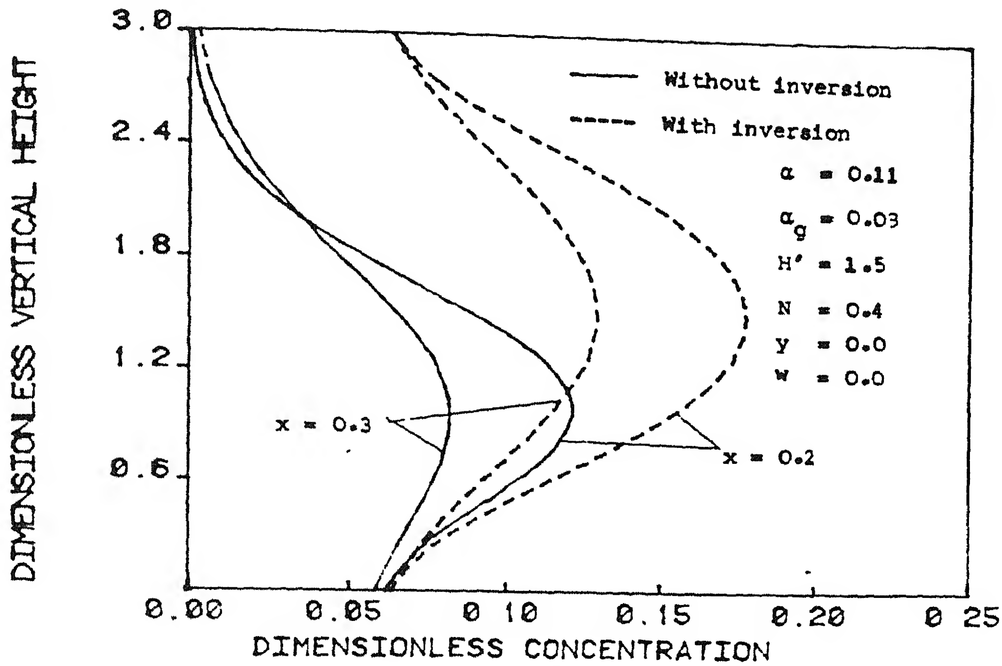

FIG 5.15 VERTICAL CONCENTRATION PROFILE FOR DIFFERENT X

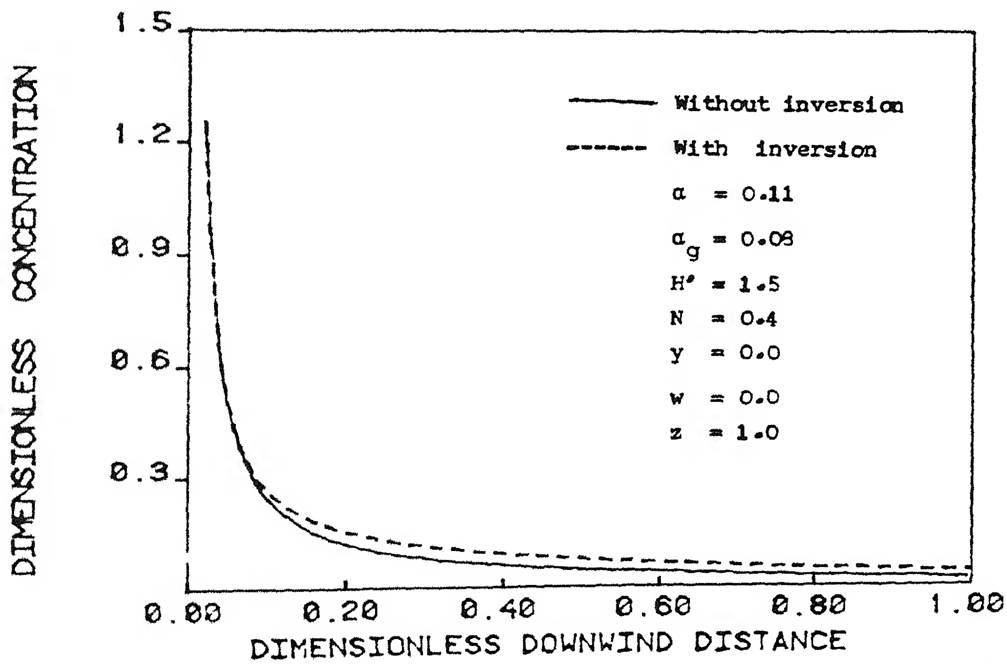

FIG 5.16 DOWNWIND DISTANCE CONCENTRATION PROFILE AT Z = 1.0

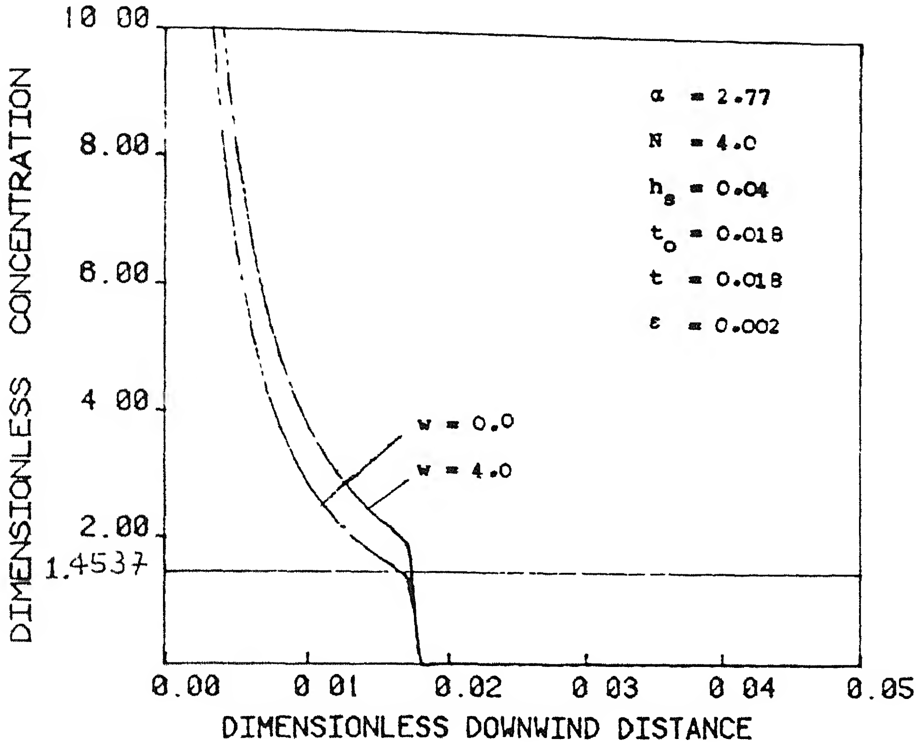

FIG 5.17

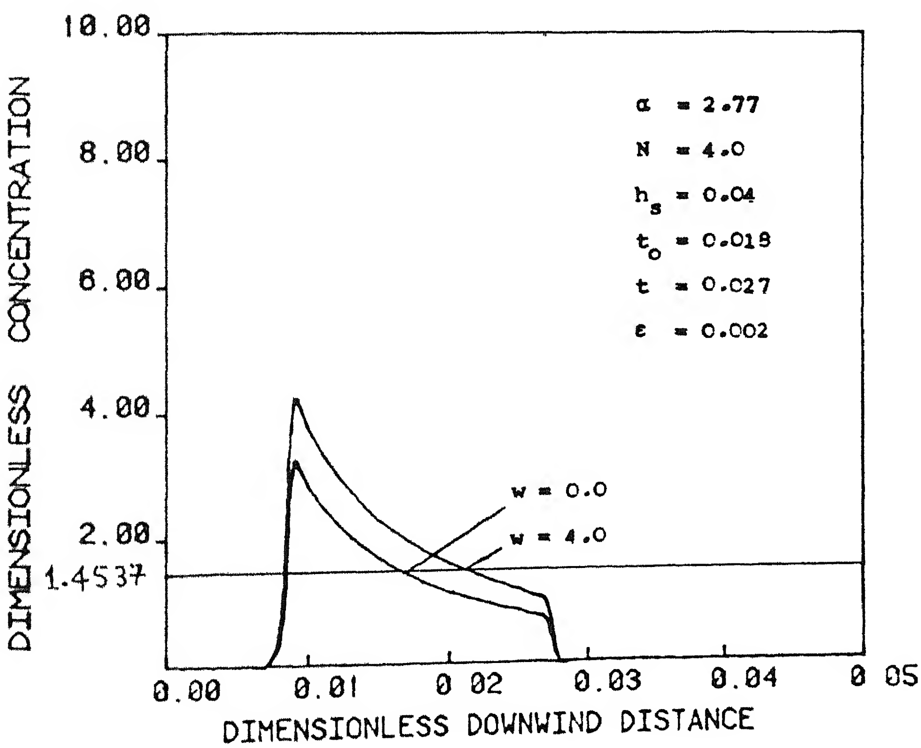

FIG 5 18

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CHAPTER VI

EFFECT OF VARIABLE WIND VELOCITY AND DIFFUSIVITIES ON DISPERSION OF AIR POLLUTANT FROM POINT AND LINE SOURCES

6.1 INTRODUCTION

The unsteady dispersion of air pollutant from a time dependent point source under going first order chemical reaction forming secondary pollutant has been discussed in chapters II-V. The analytical solution of unsteady state three dimensional diffusion equation has been obtained by taking into account first order chemical kinetics, dry and wet depositionsin chapters IV and V. It is noted here that in these studies the wind velocity and diffusion coefficients have been taken as constant. In general, however, the wind velocity and diffusivities are functions of space coordinates and time, but in the case when horizontal homogenity is assumed, the wind speed and diffusion coefficients may be taken as function of height only. In a few cases when the wind speed and diffusion coefficients are power law functions of height, the analytical solution of steady state two dimensional diffusion equation for non-reactive pollutant has been obtained when the ground surface is acting as a reflecting plane (Smith, 1957, Demuth, 1978, Robson 1983). For general functional forms of wind velocity

and diffusivities no exact solution of three dimensional diffusion equation with chemical and other removal mechanisms is known. Since a general function can be approximated by a set of step functions, one way to study this kind of problems is to divide the atmospheric layer into several layers such that the diffusion coefficients and wind velocity are taken constants but different in different layers. The diffusion equation is then solved in each layer by using these constant values with appropriate matching conditions at interfaces of these hypothetical layers.

In view of this, in this chapter, the steady state dispersion of reactive air pollutant emitted from point and line sources has been discussed by taking into account dry deposition and under the chemical reaction inversion condition and dividing the inversion layer into two, and three layers.

6.2 BASIC EQUATIONS AND SOLUTIONS

(1) TWO LAYERED MODEL

(a) Point Source

Consider the dispersion of a reactive air pollutant from a continuous point source located at height h_s above the ground in presence of an inversion layer ($0 \leq z \leq H$) of height H divided into two layers: I ($0 \leq z \leq h_g$) and

II ($h_g \leq z \leq H$), h_g being height of lower layer. When x-axis is taken along the wind direction, the steady state diffusion equation governing the concentration of the pollutant in each region, can be written as follows

Region I ($0 \leq z \leq h_g$)

$$u_1 \frac{\partial C_1}{\partial x} = K_{z1} \frac{\partial^2 C_1}{\partial z^2} + K_{y1} \frac{\partial^2 C_1}{\partial y^2} - kC_1 \tag{6.1}$$

and boundary conditions are

(i) at $x = 0$ $C_1 = 0$ (6.2)

(ii) $C_1 = 0$ as $y \to \pm \infty$ (6.3)

(iii) $K_{z1} \frac{\partial C_1}{\partial z} = v_d C_1$ at $z = 0$ (6.4)

(iv) $K_{z1} \frac{\partial C_1}{\partial z} = K_{22} \frac{\partial C_2}{\partial z}$; $C_1 = C_2$ at $z = h_g$ (6.5)

Region II ($hg \leq z \leq H$)

$$u_2 \frac{\partial C_2}{\partial x} = K_{z2} \frac{\partial^2 C_2}{\partial z^2} + K_{y2} \frac{\partial^2 C_2}{\partial y^2} - kC_2 \tag{6.6}$$

and boundary conditions are

(i) $C_2 = \frac{W}{u_2} \delta(y)\, \delta(z-h_s)$ at $x=0$ (6.7)

(ii) $C_2 = 0$ as $y \to \pm \infty$ (6.8)

(iii) $\frac{\partial C_2}{\partial z} = 0$ at $z=H$ (6.9)

(iv) $K_{z2} \frac{\partial C_2}{\partial z} = K_{z1} \frac{\partial C_1}{\partial z}$; $C_2 = C_1$ at $z = h_g$ (6.10)

where C_1, C_2 are the concentration of pollutant in the two regions, u_1, u_2 are the mean velocities, K_{y1}, K_{y2} and K_{z1}, K_{z2} are diffusion coefficients in y- and z-directions respectively. v_d is deposition velocity on the ground, k is chemical reaction rate and $\delta(.)$ is Dirac delta function and W is source strength.

If the source lies in the first region, the boundary condition at the source for equation (6.1) and (6.6) are

$$C_1 = \frac{W}{u_1}\,\delta(y)\,\delta(z-h_s) \quad \text{at} \quad x = 0 \tag{6.11}$$

$$C_2 = 0 \quad \text{at} \quad x = 0 \tag{6.12}$$

Using following dimensionless quantities

$$\bar{x} = \frac{K_{zmax}x}{u_{max}H^2}, \quad \bar{z} = \frac{z}{H}, \quad \bar{u}_i = \frac{u_i}{u_{max}}, \quad \bar{y} = \frac{y}{H}$$

$$\bar{K}_{zi} = \frac{K_{zi}}{K_{zmax}}, \quad \bar{v}_d = \frac{v_d H}{K_{zmax}}, \quad \bar{h}_g = \frac{h_g}{H}, \quad \bar{h}_s = \frac{h_s}{H} \tag{6.13}$$

$$\bar{C}_i = \frac{u_{max}H^2}{W}\,C_i, \quad (i = 1, 2)$$

equations (6.1 - 6.12) become

Region I $(0 \leq \bar{z} \leq \bar{h}_g)$

$$\frac{\partial \bar{C}_1}{\partial \bar{x}} = \beta_1 \frac{\partial^2 \bar{C}_1}{\partial \bar{y}^2} + \gamma_1 \frac{\partial^2 \bar{C}_1}{\partial \bar{z}^2} - \alpha_1 \bar{C}_1 \tag{6.14}$$

$$\bar{C}_1 = 0 \quad \text{at} \quad \bar{x} = 0 \tag{6.15}$$

$$\bar{C}_1 = 0 \text{ as } \bar{y} \to \pm\infty \tag{6.16}$$

$$\frac{\partial \bar{C}_1}{\partial \bar{z}} = N_1 \bar{C}_1 \quad \text{at} \quad \bar{z} = 0 \tag{6.17}$$

$$\bar{K}_{z1} \frac{\partial \bar{C}_1}{\partial \bar{z}} = \bar{K}_{z2} \frac{\partial \bar{C}_2}{\partial \bar{z}}, \quad \bar{C}_1 = \bar{C}_2 \text{ at } \bar{z} = \bar{h}_g \tag{6.18}$$

Region II ($\bar{h}_g \leq \bar{z} \leq 1$)

$$\frac{\partial \bar{C}_2}{\partial \bar{x}} = \beta_2 \frac{\partial^2 \bar{C}_2}{\partial \bar{y}^2} + \gamma_2 \frac{\partial^2 \bar{C}_2}{\partial \bar{z}^2} - \alpha_2 \bar{C}_2 \tag{6.19}$$

$$\bar{C}_2 = \frac{1}{\bar{u}_2} \delta(\bar{y})\, \delta(\bar{z}-\bar{h}_s) \quad \text{at} \quad \bar{x} = 0 \tag{6.20}$$

$$\bar{C}_2 = 0 \quad \bar{y} \to \pm\infty \tag{6.21}$$

$$\frac{\partial \bar{C}_2}{\partial \bar{z}} = 0 \quad \text{at} \quad \bar{z} = 1 \tag{6.22}$$

$$\bar{K}_{z2} \frac{\partial \bar{C}_2}{\partial \bar{z}} = \bar{K}_{z1} \frac{\partial \bar{C}}{\partial \bar{z}}, \quad \bar{C}_1 = \bar{C}_2 \quad \text{at} \quad \bar{z} = \bar{h}_g \tag{6.23}$$

where

$$\gamma_1 = \frac{\bar{K}_{z1}}{\bar{u}_1}, \quad \gamma_2 = \frac{\bar{K}_{z2}}{\bar{u}_2}, \quad \alpha_1 = \frac{\alpha}{\bar{u}_1}, \quad \alpha_2 = \frac{\alpha}{\bar{u}_2}$$

$$N_1 = \frac{\bar{v}_d}{\bar{K}_{z1}}, \quad \beta_1 = \frac{K_{y1}}{\bar{u}_1 K_{zmax}}, \quad \beta_2 = \frac{K_{y2}}{\bar{u}_2 K_{zmax}}$$

$$\alpha = \frac{kH^2}{K_{zmax}}$$

$$K_{zmax} = \max(K_{z1}, K_{z2}), \quad u_{max} = \max(u_1, u_2).$$

The solutions of equations (6.14) and (6.19) are obtained by using Fourier transform, with the assumption $\beta_1 = \beta_2$ i.e. $\frac{K_{y1}}{u_1} = \frac{K_{y2}}{u_2}$ (dropping bars for convenience) as

$$C_1(x,y,z) = \frac{e^{-(y^2/4\beta_1 x)}}{\sqrt{4\pi\beta_1 x}} \sum_{n=1}^{\infty} e^{-\delta_n^2 x} R_n \frac{\left(\frac{N_1}{a_{11n}} \sin a_{11n}z + \cos a_{11n}z\right)}{\left(\frac{N_1}{a_{11n}} \sin a_{11n}h_g + \cos a_{11n}h_g\right)} \tag{6.24}$$

$$C_2(x,y,z) = \frac{e^{-(y^2/4\beta_1 x)}}{\sqrt{4\pi\beta_1 x}} \sum_{n=1}^{\infty} e^{-\delta_n^2 x} R_n \frac{(\tan a_{12n} \sin a_{12n}z + \cos a_{12n}z)}{(\tan a_{12n} \sin a_{12n}h_g + \cos a_{12n}h_g)} \tag{6.25}$$

where

$$R_n = \frac{(\tan a_{12n} \sin a_{12n} h_s + \cos a_{12n}h_s)}{F(\tan a_{12n} \sin a_{12n} h_g + \cos a_{12n}h_g)}$$

$$F = \frac{u_1 P_1^2}{4a_{11n}} \Big[2a_{11n} h_g \left(1 + \frac{N_1^2}{a_{11n}^2}\right) + \left(1 - \frac{N_1^2}{a_{11n}^2}\right) \sin 2a_{11n}h_g$$

$$- \frac{2N_1}{a_{11n}} (\cos 2a_{11n}h_g - 1) \Big]$$

$$+ \frac{u_2 P_2^2}{4a_{12n}} \Big[2a_{12n}(1-h_g)(1 + \tan^2 a_{12n})$$

$$+ (1 - \tan^2 a_{12n})(\sin 2a_{12n} - \sin 2a_{12n}h_g)$$

$$- 2 \tan a_{12n}(\cos 2a_{12n} - \cos 2a_{12n} h_g) \Big]$$

$$a_{11n} = \sqrt{\frac{\delta_n^2 - \alpha_1}{\gamma_1}}, \quad a_{12n} = \sqrt{\frac{\delta_n^2 - \alpha_2}{\gamma_2}}$$

$$P_1 = 1/\left(\frac{N_1}{a_{11n}} \sin a_{11n} h_g + \cos a_{11n} h_g\right)$$

$$P_2 = 1/(\tan a_{12n} \sin a_{12n} h_g + \cos a_{12n} h_g)$$

and δ_n's are the solutions of following transcedental equation:

$$K_{z1} \frac{(N_1 \cos a_{11} h_g - a_{11} \sin a_{11} h_g)}{\left(\frac{N_1}{a_{11}} \sin a_{11} h_g + \cos a_{11} h_g\right)}$$

$$= \frac{K_{z2}(a_{12} \tan a_{12} \cos a_{12} h_g - a_{12} \sin a_{12} h_g)}{(\tan a_{12} \sin a_{12} h_g + \cos a_{12} h_g)} \qquad (6.26)$$

Now, if the source lies in first region, the concentration of pollutant in different regions is given by

$$C_1(x,y,z) = \frac{e^{-\left(\frac{y^2}{4\beta_1 x}\right)}}{\sqrt{4\beta_1 \pi x}} \sum_{n=1}^{\infty} e^{-\delta_n^2 x} R_{no} \frac{\left(\frac{N_1}{a_{11n}} \sin a_{11n} z + \cos a_{11n} z\right)}{\left(\frac{N_1}{a_{11n}} \sin a_{11n} h_g + \cos a_{11n} h_g\right)}$$

(6.27)

$$C_2(x,y,z) = \frac{e^{-\left(\frac{y^2}{4\beta_1 x}\right)}}{\sqrt{4\beta_1 \pi x}} \sum_{n=1}^{\infty} e^{-\delta_n^2 x} R_{no} \frac{(\tan a_{12n} \sin a_{12n} z + \cos a_{12n} z)}{(\tan a_{12n} \sin a_{12n} h_g + \cos a_{12n} h_g)}$$

(6.28)

where

$$R_{no} = \frac{\left(\frac{N_1}{a_{11n}} \sin a_{11n} h_s + \cos a_{11n} h_s\right)}{F(\tan a_{12n} \sin a_{12n} h_g + \cos a_{12n} h_g}$$

and F is defined above.

(b) Infinite Line Source

Consider the dispersion of a reactive air pollutant from a continuous infinite line source in the two layered inversion region as before. In this case, the partial differential equations governing the concentration of pollutant in each region are,

Region I $(0 \leq z \leq h_g)$

$$u_1 \frac{\partial C_1}{\partial x} = K_{z1} \frac{\partial^2 C_1}{\partial z^2} - kC_1 \qquad (6.29)$$

with boundary conditions

(i) $C_1 = 0$ at $x = 0$ (6.30)

(ii) $K_{z1} \frac{\partial C_1}{\partial z} = v_d C_1$ at $z = 0$ (6.31)

(iii) $K_{z1} \frac{\partial C_1}{\partial z} = K_{z2} \frac{\partial C_2}{\partial z}$, $C_1 = C_2$ at $z=h_g$ (6.32)

Region II $(h_g \leq z \leq H)$

$$u_2 \frac{\partial C_2}{\partial x} = K_{z2} \frac{\partial^2 C_2}{\partial z^2} - kC_2 \qquad (6.33)$$

(i) $$C_2 = \frac{W}{u_2}\,\delta(z-h_s) \quad \text{at } x = 0 \tag{6.34}$$

(ii) $$\frac{\partial C_2}{\partial z} = 0 \quad \text{at } z = H \tag{6.35}$$

(iii) $$K_{z2}\frac{\partial C_2}{\partial z} = K_{z1}\frac{\partial C_1}{\partial z} \qquad C_2 = C_1 \ \text{at } z = h_g\,. \tag{6.36}$$

If the source lies in the first layer, the boundary conditions at the source for equations (6.29) and (6.33) are

$$C_1 = \frac{W}{u_1}\,\delta(z-h_s) \quad \text{at } x = 0 \tag{6.37}$$

$$C_2 = 0 \qquad \text{at } x = 0. \tag{6.38}$$

The solution of equations (6.29) and (6.33) subjected to above boundary conditions can be obtained as before and written in the dimensionless form, for each region, as follows:

$$C_1(x,z) = \sum_{n=1}^{\infty} R_n e^{-\delta_n^2 x}\,\frac{\left(\frac{N_1}{a_{11n}}\sin a_{11n}z + \cos a_{11n}z\right)}{\left(\frac{N_1}{a_{11n}}\sin a_{11n}h_g + \cos a_{11n}h_g\right)} \tag{6.39}$$

$$C_2(x,z) = \sum_{n=1}^{\infty} R_n e^{-\delta_n^2 x}\,\frac{(\tan a_{12n}\sin a_{12n}z + \cos a_{12n}z)}{(\tan a_{12n}\sin a_{12n}h_g + \cos a_{12n}h_g)} \tag{6.40}$$

When the source lies in the first region, the corresponding dimensionless distributions of $C_1(x,z)$ and $C_2(x,z)$ are given as follows:

$$C_1(x,z) = \sum_{n=1}^{\infty} R_{no} e^{-\delta_n^2 x} \frac{(\frac{N_1}{a_{11n}} \sin a_{11n}z + \cos a_{11n}z)}{(\frac{N_1}{a_{11n}} \sin a_{11n}h_g + \cos a_{11n}h_g)} \quad (6.42)$$

$$C_2(x,z) = \sum_{n=1}^{\infty} R_{no} e^{-\delta_n^2 x} \frac{(\tan a_{12n}\cos a_{12n}z+\sin a_{12n}z)}{(\tan a_{12n}\sin a_{12n}h_g+\cos a_{12n}h_g)} \quad (6.42)$$

where various parameters are same as defined in the case of point source.

It is also noted that equations (6.39)-(6.42) can be obtained by integrating equations (6.24)-(6.28) with respect to y between $-\infty$ and ∞ respectively.

(ii) THREE LAYERED MODEL

(a) Point Source

Consider the dispersion of a reactive air pollutant from a continuous point source of strength W, located at height h_s above the ground in the second region of the inversion layer which is divided into three layers: I $(0 \leq z \leq h_1)$, II $(h_1 \leq z \leq h_2)$ and III $(h_2 \leq z \leq H)$. The steady state diffusion equation governing the concentration of the pollutant in each region can be written as follows:

Region I $(0 \leq z \leq h_1)$

$$u_1 \frac{\partial C_1}{\partial x} = k_{y1} \frac{\partial^2 C_1}{\partial y^2} + k_{z1} \frac{\partial^2 C_1}{\partial z^2} - k\, C_1 \quad (6.43)$$

with boundary conditions

(i) $C_1 = 0$ at $x = 0$ (6.44)

(ii) $C_1 = 0$ at $y \to \pm \infty$ (6.45)

(iii) $K_{z1} \dfrac{\partial C_1}{\partial z} = v_d C_1$ at $z = 0$ (6.46)

(iv) $K_{z1} \dfrac{\partial C_1}{\partial z} = K_{z2} \dfrac{\partial C_2}{\partial z}$, $C_1 = C_2$ at $z = h_1$ (6.47)

Region II ($h_1 \leq z \leq h_2$)

$$u_2 \frac{\partial C_2}{\partial x} = K_{y2} \frac{\partial^2 C_2}{\partial y^2} + K_{z2} \frac{\partial^2 C_2}{\partial z^2} - kC_2 \tag{6.48}$$

with boundary conditions

(i) $C_2 = \dfrac{W}{u_2} \delta(y) \delta(z - h_s)$ at $x = 0$ (6.49)

(ii) $C_2 = 0$ as $y \to \pm \infty$ (6.50)

(iii) $K_{z2} \dfrac{\partial C_2}{\partial z} = K_{z1} \dfrac{\partial C_1}{\partial z}$, $C_2 = C_1$ at $z = h_1$ (6.51)

(iv) $K_{z2} \dfrac{\partial C_2}{\partial z} = K_{z3} \dfrac{\partial C_3}{\partial z}$, $C_2 = C_3$ at $z = h_2$ (6.52)

Region III ($h_2 \leq z \leq H$)

$$u_3 \frac{\partial C_3}{\partial x} = K_{y3} \frac{\partial^2 C_3}{\partial y^2} + K_{z3} \frac{\partial^2 C_3}{\partial z^2} - kC_3 \tag{6.53}$$

with boundary conditions

(i) $C_3 = 0$ at $x = 0$ (6.54)

(ii) $C_3 = 0$ as $y \to \pm \infty$ (6.55)

(iii) $K_{z3} \dfrac{\partial C_3}{\partial z} = K_{z2} \dfrac{\partial C_3}{\partial z}$, $C_3 = C_2$ at $z=h_2$ (6.56)

(iv) $\dfrac{\partial C_3}{\partial z} = 0$ at $z = H$ (6.57)

If the source lies in the first region, the boundary conditions at the source for equations (6.43), (6.48) and (6.53) are

$$C_1 = \frac{W}{u_1} \delta(u)\delta(z-h_s) \quad \text{at } x = 0$$

$$C_2 = 0 \quad \text{at } x = 0 \tag{6.58}$$

$$C_3 = 0 \quad \text{at } x = 0$$

Using following dimensionless quantities

$$\bar{x} = \frac{K_{zmax}x}{u_{max}H^2}, \quad \bar{z} = \frac{z}{H}, \quad \bar{u}_i = \frac{u_i}{u_{max}}, \quad \bar{y} = \frac{y}{H}$$

$$\bar{K}_{zi} = \frac{K_{zi}}{K_{zmax}}, \quad \bar{v}_d = \frac{v_d H}{K_{zmax}}, \quad \bar{h}_i = \frac{h_i}{H}, \quad \bar{h}_s = \frac{h_s}{H} \tag{6.59}$$

$$\bar{C}_i = \frac{u_{max}H^2}{W} C_i \quad (i=1,2,3)$$

equations (6.43)-(6.57) can be written, in the dimensionless form as

Region I ($0 \le \bar{z} \le \bar{h}_1$)

$$\frac{\partial \bar{C}_1}{\partial \bar{x}} = \beta_1 \frac{\partial^2 \bar{C}_1}{\partial \bar{y}^2} + \gamma_1 \frac{\partial^2 \bar{C}_1}{\partial \bar{z}^2} - \alpha_1 \bar{C}_1 \tag{6.60}$$

$$\bar{C}_1 = 0 \quad \text{at} \quad \bar{x} = 0 \tag{6.61}$$

$$\bar{C}_1 = 0 \quad \text{as} \quad \bar{y} \to \pm \infty \tag{6.62}$$

$$\frac{\partial \bar{C}_1}{\partial \bar{z}} = N_1 \bar{C}_1 \quad \text{at} \quad \bar{z} = 0 \tag{6.63}$$

$$\bar{K}_{z1} \frac{\partial \bar{C}_1}{\partial \bar{z}} = \bar{K}_{z2} \frac{\partial \bar{C}_2}{\partial \bar{z}}, \quad \bar{C}_1 = \bar{C}_2 \quad \text{at} \quad \bar{z} = \bar{h}_1 \tag{6.64}$$

Region II ($\bar{h}_1 \leq \bar{z} \leq \bar{h}_2$)

$$\frac{\partial \bar{C}_2}{\partial \bar{x}} = \beta_2 \frac{\partial^2 \bar{C}_2}{\partial \bar{y}^2} + \gamma_2 \frac{\partial^2 \bar{C}_2}{\partial \bar{z}^2} - \alpha_2 \bar{C}_2 \tag{6.65}$$

$$\bar{C}_2 = \frac{1}{\bar{u}_2} \delta(\bar{y}) \, \delta(\bar{z}-\bar{h}_s) \quad \text{at} \quad \bar{x} = 0 \tag{6.66}$$

$$\bar{C}_2 = 0 \quad \text{as} \quad \bar{y} \to \pm \infty \tag{6.67}$$

$$\bar{K}_{z2} \frac{\partial \bar{C}_2}{\partial \bar{z}} = \bar{K}_{z1} \frac{\partial \bar{C}_1}{\partial \bar{z}}, \quad \bar{C}_1 = \bar{C}_2 \quad \text{at} \quad \bar{z} = \bar{h}_1 \tag{6.68}$$

$$\bar{K}_{z2} \frac{\partial \bar{C}_2}{\partial \bar{z}} = \bar{K}_{z3} \frac{\partial \bar{C}_3}{\partial \bar{z}}, \quad \bar{C}_2 = \bar{C}_3 \quad \text{at} \quad \bar{z} = \bar{h}_2 \tag{6.69}$$

Region III ($\bar{h}_2 \leq \bar{z} \leq 1$)

$$\frac{\partial \bar{C}_3}{\partial \bar{x}} = \beta_3 \frac{\partial^2 \bar{C}_3}{\partial \bar{y}^2} + \gamma_3 \frac{\partial^2 \bar{C}_3}{\partial \bar{z}^2} - \alpha_3 \bar{C}_3 \tag{6.70}$$

$$\bar{C}_3 = 0 \quad \text{at} \quad \bar{x} = 0 \tag{6.71}$$

$$\bar{C}_3 = 0 \quad \text{as} \quad \bar{y} \to \pm \infty \tag{6.72}$$

$$\bar{K}_{z3}\frac{\partial \bar{C}_3}{\partial \bar{z}} = \bar{K}_{z2}\frac{\partial \bar{C}_2}{\partial \bar{z}}, \quad \bar{C}_3 = \bar{C}_2 \text{ at } \bar{z} = \bar{h}_2 \tag{6.73}$$

$$\frac{\partial \bar{C}_3}{\partial \bar{z}} = 0 \qquad \text{at } \bar{z} = 1 \tag{6.74}$$

where

$$\gamma_i = \frac{\bar{K}_{zi}}{\bar{u}_i}, \quad \alpha_i = \frac{\alpha}{\bar{u}_i}, \quad \alpha = \frac{kH^2}{K_{zmax}}, \quad N_1 = \frac{\bar{v}_d}{\bar{K}_{z1}}, \quad \beta_i = \frac{K_{yi}}{K_{zmax}\bar{u}_i}$$

$(i=1, 2, 3)$

$$K_{zmax} = \max(K_{z1}, K_{z2}, K_{z3}) \quad u_{max} = \max(u_1, u_2, u_3).$$

The solutions of equations (6.60), (6.65) and (6.70) with the assumption $\beta_1=\beta_2=\beta_3$ i.e. $\frac{K_{y1}}{u_1} = \frac{K_{y2}}{u_2} = \frac{K_{y3}}{u_3}$, can be written (dropping bars for convenience) as

$$C_1(x,y,z) = \frac{e^{-\left(\frac{y^2}{4\beta_1 x}\right)}}{2\sqrt{\pi\beta_1 x}} \sum_{n=1}^{\infty} R_{n1}\, e^{-\delta_n'^2 x}\, G_{1n}(z) \tag{6.75}$$

$$C_2(x,y,z) = \frac{e^{-\left(\frac{y^2}{4\beta_1 x}\right)}}{2\sqrt{\pi\beta_1 x}} \sum_{n=1}^{\infty} R_{n1}\, e^{-\delta_n'^2 x}\, G_{1n}(z) \tag{6.76}$$

$$C_3(x,y,z) = \frac{e^{-\left(\frac{y^2}{4\beta_1 x}\right)}}{2\sqrt{\pi\beta_1 x}} \sum_{n=1}^{\infty} R_{n1}\, e^{-\delta_n'^2 x}\, G_{3n}(z) \tag{6.77}$$

$$G_{1n}(z) = P_3\left(\frac{N_1}{a'_{11n}} \sin a'_{11n}z + \cos a'_{11n}z\right)$$

$$G_{2n}(z) = P_4(R \sin a'_{12n}z + \cos a'_{12n}z)$$

$$G_{3n}(z) = P_5 \ (\tan a'_{13n} \sin a'_{13n}z + \cos a'_{13n}z)$$

$$P_3 = 1/(N_1/a'_{11n} \sin a'_{11n}h_1 + \cos a'_{11n}h_1)$$

$$P_4 = 1/(R \sin a'_{12n}h_1 + \cos a'_{12n}h_1)$$

$$P_5 = \frac{(R \sin a'_{12n}h_2 + \cos a'_{12n}h_2)P_4}{(\tan a'_{13n} \sin a'_{13n}h_2 + \cos a'_{13n}h_2)}$$

$$R = \frac{\begin{array}{l} K_{z2}a'_{12}\sin a'_{12}h_2(\tan a'_{13}\sin a'_{13}h_2 + \cos a'_{13}h_2) \\ \qquad + K_{z3}\cos a'_{12}h_2(a'_{13}\tan a'_{13}\cos a'_{13}h_2 - a'_{13}\sin a'_{13}h_2) \end{array}}{\begin{array}{l} K_{z2}a'_{12}\cos a'_{12}h_2(\tan a'_{13}\sin a'_{13}h_2 + \cos a'_{13}h_2) \\ \qquad + K_{z3}\sin a'_{12}h_2(a'_{13}\tan a'_{13}\cos a'_{13}h_2 - a'_{13}\sin a'_{13}h_2) \end{array}}$$

$$R_{n1} = \frac{G_{2n}(h_s)}{F_1}$$

$$F_1 = \frac{u_1P_3^2}{4a'_{11n}}\left[\left(1 - \frac{N_1^2}{a'^2_{11n}}\right)\sin 2a'_{11n}h_1 + 2a'_{11n}\left(1 + \frac{N_1^2}{a'^2_{11n}}\right)h_1 - \frac{2N_1}{a'_{11n}}(\cos 2a'_{11n}h_1 - 1)\right]$$

$$+ \frac{u_2P_4^2}{4a'_{12n}}\left[(1-R^2)\{\sin 2a'_{12n}h_2 - \sin 2a'_{12n}h_1\} + 2a'_{12n}(1+R^2)(h_2-h_1) - 2R(\cos 2a'_{12n}h_2 - \cos 2a'_{12n}h_1)\right]$$

$$+\frac{u_3 P_5^2}{4a'_{13n}}\Big[(1-\tan^2 a'_{13n})(\sin 2a'_{13n}-\sin 2a'_{13n}h_2)$$

$$+2a'_{13n}(1-h_2)(1+\tan^2 a'_{13n})$$

$$-2\tan a'_{13n}(\cos 2a'_{13n}-\cos 2a'_{13n}h_2)\Big]$$

$$a'_{11n}=\sqrt{\frac{\delta_n'^2-\alpha_1}{\gamma_1}}\,,\quad a'_{12n}=\sqrt{\frac{\delta_n'^2-\alpha_2}{\gamma_2}}\,,\quad a'_{13n}=\sqrt{\frac{\delta_n'^2-\alpha_3}{\gamma_3}}$$

and δ'_n's are eigen values of following transcendental equation

$$\frac{\begin{aligned}&K_{z2}a'_{12}\sin a'_{12}h_1\left(\frac{N_1}{a'_{11}}\sin a'_{11}h_1+\cos a'_{11}h_1\right)\\&\qquad+K_{z1}\cos a'_{12}h_1(N_1\cos a'_{11}h_1-a'_{11}\sin a'_{11}h_1)\end{aligned}}{\begin{aligned}&K_{z2}a'_{12}\cos a'_{12}h_1\left(\frac{N_1}{a'_{11}}\sin a'_{11}h_1+\cos a'_{11}h_1\right)\\&\qquad-K_{z1}\sin a'_{12}h_1(N_1\cos a'_{11}h_1-a'_{11}\sin a'_{11}h_1)\end{aligned}}$$

$$=\frac{\begin{aligned}&K_{z2}a'_{12}\sin a'_{12}h_2(\tan a'_{13}\sin a'_{13}h_2+\cos a'_{13}h_2)\\&\qquad+K_{z3}\cos a'_{12}h_2(a'_{13}\tan a'_{13}\cos a'_{13}h_2-a'_{13}\sin a'_{13}h_2)\end{aligned}}{\begin{aligned}&K_{z2}a'_{12}\cos a'_{12}h_2(\tan a'_{13}\sin a'_{13}h_2+\cos a'_{13}h_2)\\&\qquad-K_{z3}\sin a'_{12}h_2(a'_{13}\tan a'_{13}\cos a'_{13}h_2-a'_{13}\sin a'_{13}h_2)\end{aligned}}$$

(6.78)

If the source lies in the first region, the corresponding dimensionless concentration of pollutant in each region is

$$C_1(x,y,z) = \frac{e^{-\left(\frac{y^2}{4\beta_1 x}\right)}}{2\sqrt{\pi\beta_1 x}} \sum_{n=1}^{\infty} R'_{no}\, e^{-\delta_n'^2 x}\, G_{1n}(z) \tag{6.79}$$

$$C_2(x,y,z) = \frac{e^{-\left(\frac{y^2}{4\beta_1 x}\right)}}{2\sqrt{\pi\beta_1 x}} \sum_{n=1}^{\infty} R'_{no}\, e^{-\delta_n'^2 x}\, G_{2n}(z) \tag{6.80}$$

$$C_3(x,y,z) = \frac{e^{-\left(\frac{y^2}{4\beta_1 x}\right)}}{2\sqrt{\pi\beta_1 x}} \sum_{n=1}^{\infty} R'_{no}\, e^{-\delta_n'^2 x}\, G_{3n}(z) \tag{6.81}$$

$$R'_{no} = \frac{G_{1n}(h_s)}{F_1} .$$

(b) Infinite Line Source

In this case the concentration of pollutant, when the source lies in second region, is obtained by integrating equations (6.75)-(6.77) with respect to y between $-\infty$ to ∞ and written as

$$C_1(x,z) = \sum_{n=1}^{\infty} R_{n1}\, e^{-\delta_n'^2 x}\, G_{1n}(z) \tag{6.82}$$

$$C_2(x,z) = \sum_{n=1}^{\infty} R_{n1}\, e^{-\delta_n'^2 x}\, G_{2n}(z) \tag{6.83}$$

$$C_3(x,z) = \sum_{n=1}^{\infty} R_{n1}\, e^{-\delta_n'^2 x}\, G_{3n}(z) \tag{6.84}$$

Similarly, when the source lies in first region, the concentration distribution in each region is

$$C_1(x,z) = \sum_{n=1}^{\infty} R'_{no}\, e^{-\delta_n'^2 x}\, G_{1n}(z) \tag{6.85}$$

$$C_2(x,z) = \sum_{n=1}^{\infty} R'_{no}\, e^{-\delta_n'^2 x}\, G_{2n}(z) \tag{6.86}$$

$$C_3(x,z) = \sum_{n=1}^{\infty} R'_{no}\, e^{-\delta_n'^2 x}\, G_{3n}(z) \tag{6.87}$$

6.3 RESULTS AND DISCUSSION

To study the effect of various parameters on the concentration distribution of air pollutant, the following values of parameters are chosen in the case of layered model, $u_1=0.55$, $u_2=1.0$, $k_{z1}=0.55$, $k_{z2}=1.0$, $\alpha=0.55$, $h_s=0.09$ and $h_g=0.1$, $\beta_1=10.0$.

The vertical concentration profiles of pollutant are depicted in figs. (6.1-6.4). It is found that the concentration of pollutant decreases as downwind distance increases in both point and line source cases. From these figs., it is also noted that the concentration of air pollutant decreases due to deposition on the ground as well with chemical reaction parameter. Similar results have also been obtained in the case of three layered model (graphs are not shown).

The effect of stepwise variation in the wind velocity on the concentration distribution of pollutant is shown in figs. (6.5-6.6) for $h_s=0.09$ $v_d= 2.0$, $\beta_1=10.0$ using following set of parameters.

(a) One layer

$u_1=1.0$, $K_{z1}=1.0$

$u_2=1.0$, $K_{z2}=1.0$

(b) two layer

$u_1=0.55$, $u_2=1.0$

$h_g=0.1$

$K_{z1}=1.0$, $K_{z2}=1.0$

(c) three layer

$u_1=0.55$, $u_2=0.75$, $u_3=1.0$

$h_1=0.1$ $h_2=0.3$

$K_{z1}=1.0$ $K_{z2}=1.0$, $K_{z3}=1.0$.

It is found that as the number of layers increases the concentration near the ground decreases.

The effect of stepwise variation on diffusion coefficient in z-direction are also shown in figs. 6.7-6.8, for $h_s=0.09$, $v_d=2.0$, $\beta_1=10.0$, using the following set of parameters

(a) One layer

$u_1=1.0$

$K_{z1}=1.0$

$u_2=1.0$, $K_{z2}=1.0$

(b) two layer

$u_1=1.0$, $u_2=1.0$

$h_g=0.1$

$K_{z1}=0.55$, $K_{z2}=1.0$

(c) three layer

$u_1=1.0$, $u_2=1.0$, $u_3=1.0$

$h_1=0.1$, $h_2=0.3$

$K_{z1}=0.55$, $K_{z2}=0.60$

$K_{z3}=1.0$

In this case the concentration of pollutant increases in the lower region as number of layers increases .

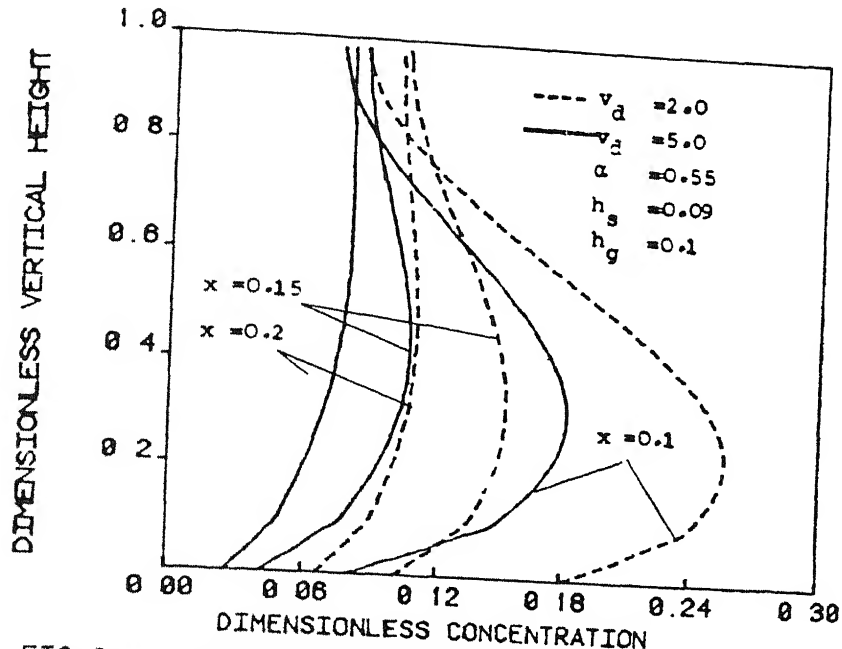

FIG 6 1 EFFECT OF DRY DEPOSITION IN THE CASE OF POINT SOURCE

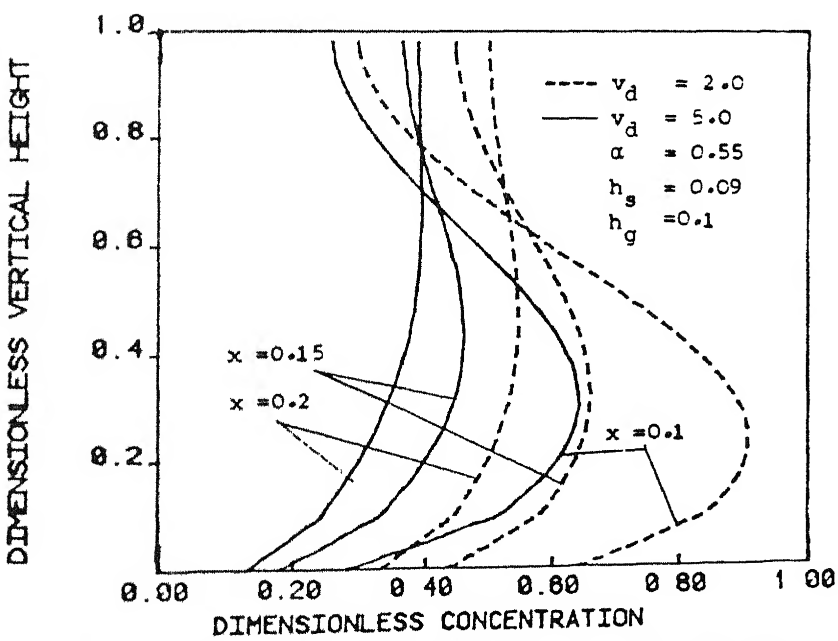

FIG 6.2 EFFECT OF DRY DEPOSITION IN THE CASE OF LINE SOURCE

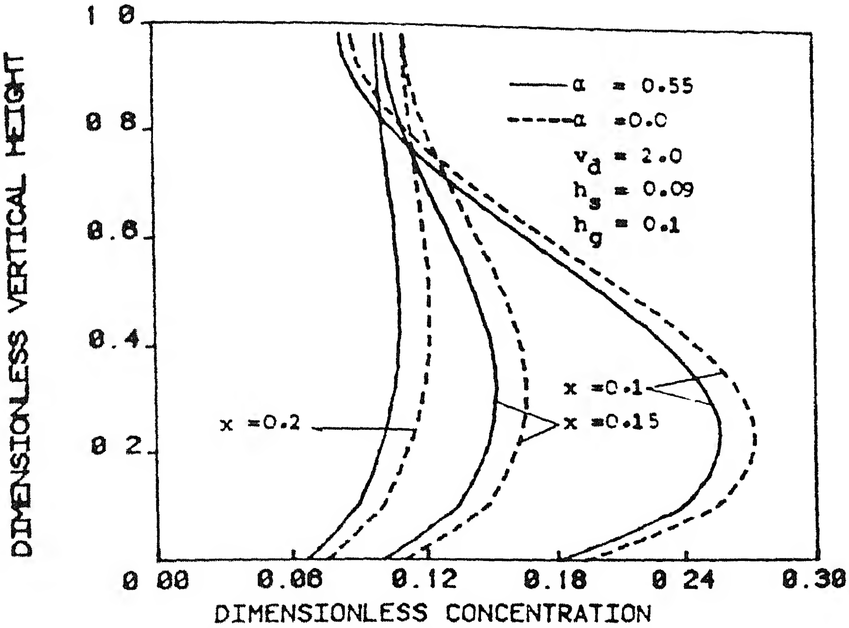

FIG 6.3 EFFECT OF CHEMICAL REACTION IN THE CASE OF POINT SOURCE

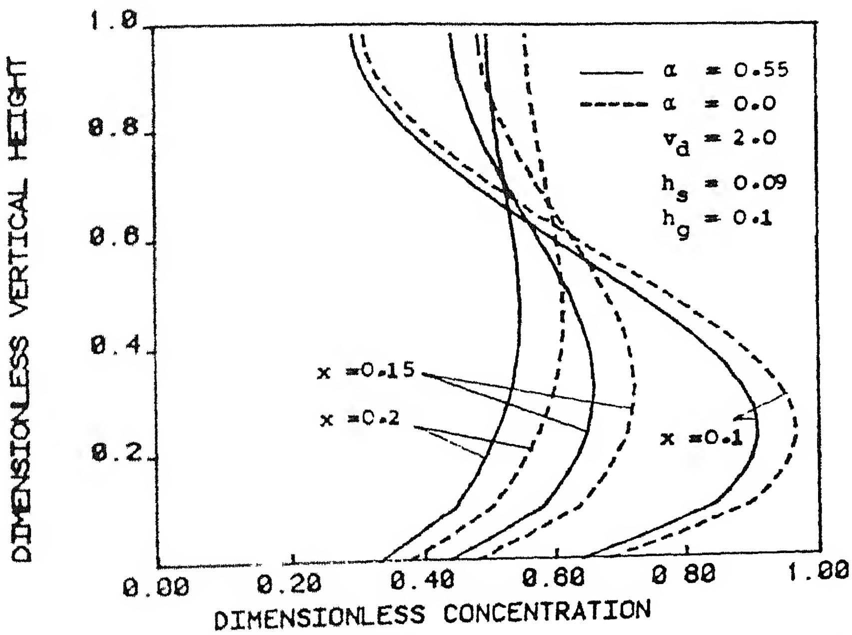

FIG 6.4 EFFECT OF CHEMICAL REACTION IN THE CASE OF LINE SOURCE

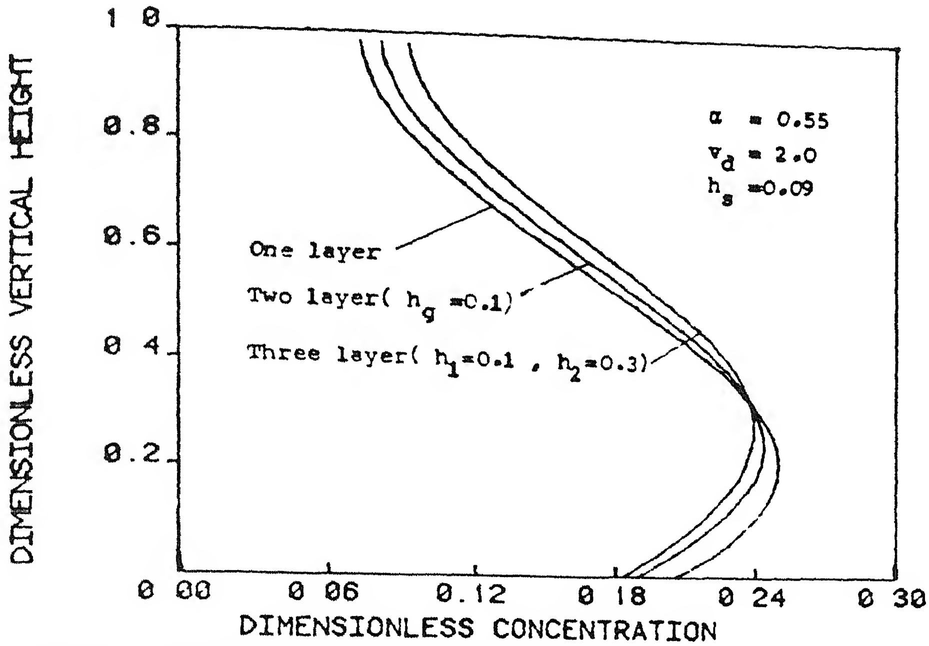

FIG 6 5 VERTICAL CONCENTRATION PROFILE AT x =0 1

EFFECT OF VARIATION OF WIND VELOCITY

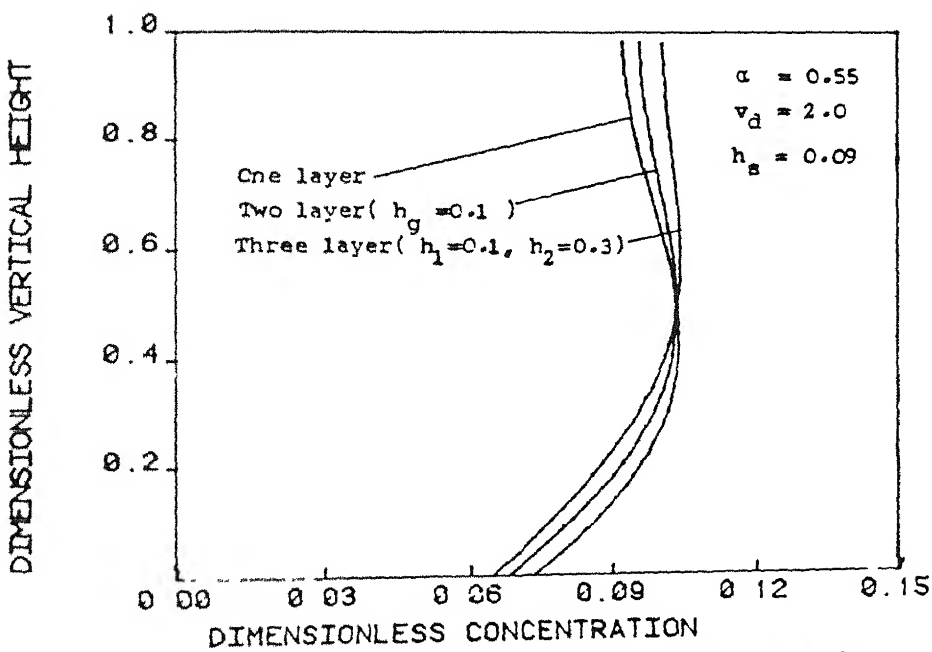

FIG 6.6 VERTICAL CONCENTRATION PROFILE FOR x =0.2

EFFECT OF THE VARIATION OF WIND VELOCITY

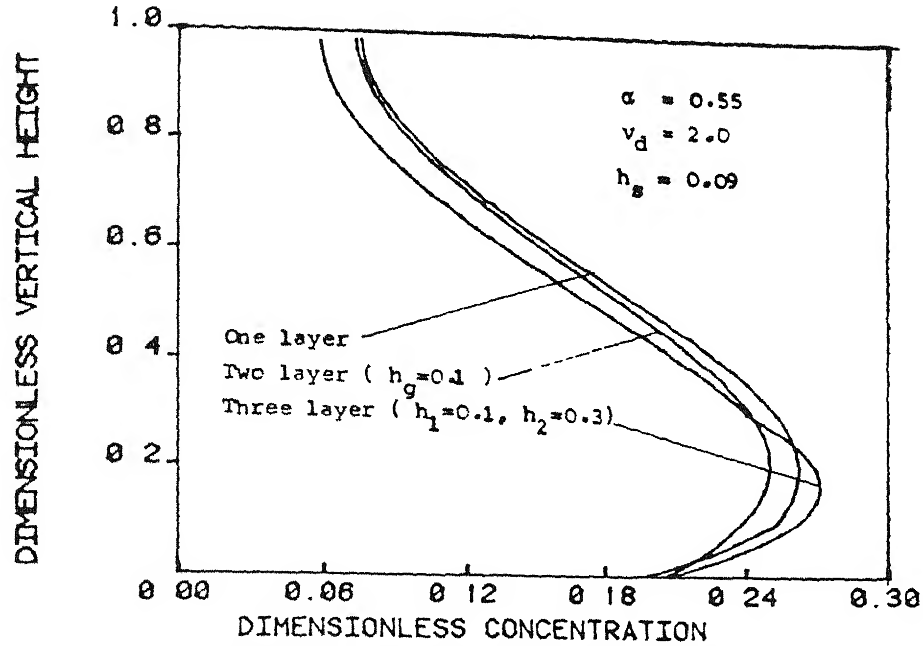

FIG6.7 VERTICAL CONCENTRATION PROFILE AT $x = 0.1$
EFFECT OF VARIATION OF DIFFUSION COEFFICIENT

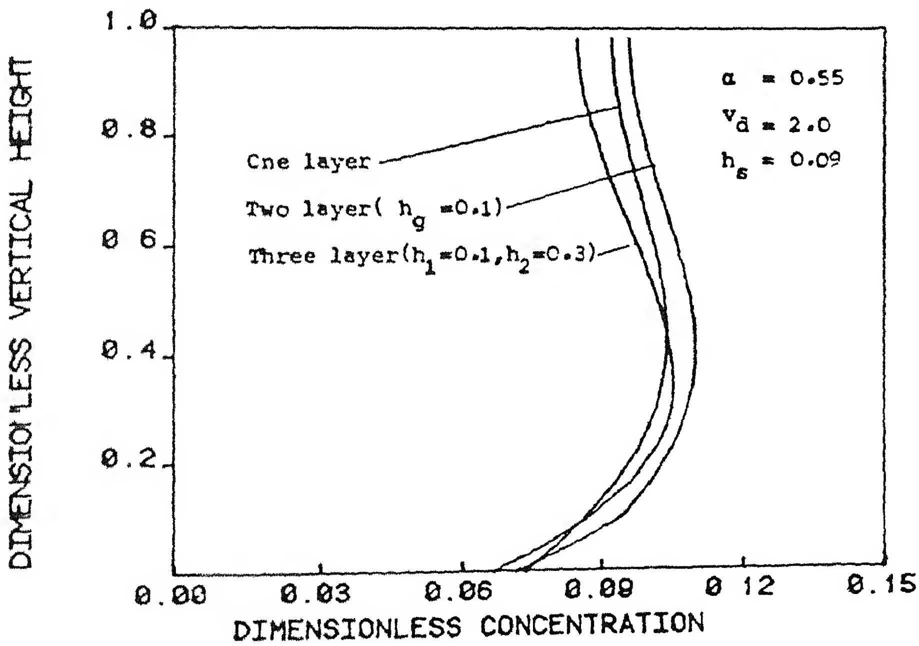

FIG 6 8 VERTICAL CONCENTRATION PRRFILE AT $x=0.2$
EFFECT OF VARIATION OF DIFFUSION COEFFICIENT

CHAPTER VII

STEADY STATE DISPERSION OF A REACTIVE AIR POLLUTANT IN PRESENCE OF GREEN BELT

7.1 INTRODUCTION

As pointed out earlier the dispersion of air pollutants is governed by the processes of molecular diffusion and convection. In the atmosphere, dispersal process depends upon the type and number of sources, stack heights, various meteorogical factors (such as wind, temperature inversion, rainout/washout) and topography of the terrain (Pasquill, 1962; Seinfeld, 1975). Several studies have been conducted to understand the process of pollutant dispersion by including some of the above mentioned factors (Smith, 1957; Pasquill, 1962; Hoffert, 1972; Slinn, 1974; Scriven and Fisher, 1975; Lamb and Seinfeld, 1973; Calder, 1977; Ermak, 1977; Alam and Seinfeld, 1981; Reda and Carmichael, 1982; Llewelyn, 1983; Karamchandani and Peters, 1983). In particular, the redistribution of a gas plume caused by reversible washout has been investigated by Slinn (1974).

The modelling of atmospheric pollution by nitrogen and sulfur dioxide has been studied recently by Alam and Seinfeld (1981) and Reda and Carmichael (1982). The development of a second generation mathematical model for urban

air pollution has been presented by Gregory et. al. (1982). The effect of foggy environment on reversible absorption of a pollutant from an area source has recently been studied by Shukla et. al. (1982).

The transport of gases and particulate matter within plant and vegetable canopies has also been studied. Petit et. al. (1976) presented results concerning characteristics of air flow within and above a forest by calculating SO_2 fluxes at the top of canopies. Bache (1979a, 1979b) used modified form of diffusion equation to study particulate transport within and above the foliage canopy. Slinn (1982) gave a theoretical framework to predict particle deposition due to vegetation by considering a variable wind velocity profile. A review of atmospheric deposition and plant assimilation of gases and particles has been presented by Smith (1957) and Hosker et al. (1982) wherein a mathematical model for aerosol depletion and deposition on forests employs a modified form of convective diffusion equation. This model develops the interaction between forest structure and open field by considering forest aerodynamics and aerosol characteristics (Wiman, 1985)).

From the above studies it may be speculated that if a suitable green belt in the form of forest is provided around the pollutant source, some distance away from source but close to the place (e.g. a habitat, a historical monument)

to be protected, then it is possible to protect the endangered area under consideration. In this direction Kapoor and Gupta (1984) studied the attenuation of an inert pollutant by a green belt under steady state conditions. In this chapter, we study the dispersion of a reactive air pollutant from point and line sources. We focus on dry deposition on the ground when the wind velocity and diffusion coefficients are functions of elevation. The exact solution of the diffusion equation with reaction term is obtained by dividing the inversion layer into four parts. Wind velocity and diffusion coefficients are taken as step functions with smaller values in the lower region than in the upper region. The effect of green belt on the reduction of concentration of pollutant due to a removal mechanism is, therefore, discussed.

7.2 MATHEMATICAL FORMULATION AND SOLUTIONS

(i) DISPERSION FROM POINT SOURCE

Consider the dispersion of a reactive air pollutant from a point source as discussed in chapter VI. Assume that a green belt (a suitable tree plantation capable of absorbing pollutant) of thickness d is located at a distance x_1 from the source along the wind direction and extending in- y direction. The physical situation is illustrated in fig. 7.1 where the inversion region is divided into four regions, the green belt being in region III. The partial differential

equations governing the concentration distribution of the air pollutant in different regions are written as follows:

Region I $(0 \leq z \leq h_g)$

$$u_1 \frac{\partial C_1}{\partial x} = K_{z1} \frac{\partial^2 C_1}{\partial z^2} + K_{y1} \frac{\partial^2 C_1}{\partial y^2} - kC_1 \tag{7.1}$$

with boundary conditions

(i) $C_1 = 0$ at $x = 0$ (7.2)

(ii) $C_1 = 0$ as $y \rightarrow \pm \infty$ (7.3)

(iii) $K_{z1} \frac{\partial C_1}{\partial z} = v_{d1} C_1$ at $z = 0$ (7.4)

(iv) $K_{z1} \frac{\partial C_1}{\partial z} = K_{z2} \frac{\partial C_2}{\partial z}$, $C_1 = C_2$ at $z = h_g$ (7.5)

Region II $(h_g \leq z \leq H)$

$$u_2 \frac{\partial C_2}{\partial x} = K_{z2} \frac{\partial^2 C_2}{\partial z^2} + K_{y2} \frac{\partial^2 C_2}{\partial y^2} - kC_2 \tag{7.6}$$

and boundary conditions are

(i) $C_2 = \frac{W}{u_2} \delta(y)\,\delta(z-h_s)$ at $x = 0$ (7.7)

(ii) $C_2 = 0$ as $y \rightarrow \pm \infty$ (7.8)

(iii) $\frac{\partial C_2}{\partial z} = 0$ at $z = H$ (7.9)

(iv) $K_{z2} \frac{\partial C_2}{\partial z} = K_{z1} \frac{\partial C_1}{\partial z}$, $C_2 = C_1$ at $z = h_g$ (7.10)

Region III $(0 \leq z \leq h_g)$ $x \geq x_1$

$$u_3 \frac{\partial C_3}{\partial x} = K_{z3} \frac{\partial^2 C_3}{\partial z^2} + K_{y3} \frac{\partial^2 C_3}{\partial y^2} - (k+\lambda) C_3 \qquad (7.11)$$

boundary conditions are

(i) $C_3 = C_1$ at $x = x_1$ (7.12)

(ii) $C_3 = 0$ as $y \to \pm \infty$ (7.13)

(iii) $K_{z3} \frac{\partial C_3}{\partial z} = K_{z4} \frac{\partial C_4}{\partial z}$, $C_3 = C_4$ at $z = h_g$ (7.14)

(iv) $K_{z3} \frac{\partial C_3}{\partial z} = v_{d_2} C_3$ at $z = 0$ (7.15)

Region IV $(h_g \leq z \leq H)$ $x \geq x_1$

$$u_4 \frac{\partial C_4}{\partial x} = K_{z4} \frac{\partial^2 C_4}{\partial z^2} + K_{y4} \frac{\partial^2 C_4}{\partial y^2} - kC_4 \qquad (7.16)$$

with boundary conditions

$C_4 = C_2$ at $x = x_1$ (7.17)

$C_4 = 0$ as $y \to \pm \infty$ (7.18)

$K_{z4} \frac{\partial C_4}{\partial z} = K_{z3} \frac{\partial C_3}{\partial z}$, $C_4 = C_3$ at $z = h_g$ (7.19)

$\frac{\partial C_4}{\partial z} = 0$ at $z = H$ (7.20)

where C_1, C_2, C_3, C_4 are concentrations of pollutant in different regions, k is rate of chemical reaction and λ is depletion rate of pollutant due to green belt.

It is convenient to cast the problem in dimensionless form. To do so we use following dimensionless quantities

$$\bar{x} = \frac{K_{zmax}x}{u_{max}H^2}, \quad \bar{z} = \frac{z}{H}, \quad \bar{u}_i = \frac{u_i}{u_{max}}, \quad \bar{y} = \frac{y}{H}$$

$$\bar{K}_{zi} = \frac{K_{zi}}{K_{zmax}}, \quad \bar{v}_{d1} = \frac{v_{d1}H}{K_{zmax}}, \quad \bar{v}_{d2} = \frac{v_{d2}H}{K_{zmax}}, \tag{7.21}$$

$$\bar{h}_g = \frac{h_g}{H}, \quad \bar{h}_s = \frac{h_s}{H}, \quad \bar{C}_i = \frac{u_{max}H^2}{W} C_i \quad (i=1,2,3,4).$$

Equations (7.1–7.20) can be written in the dimensionless form as

Region I $(0 \le \bar{z} \le \bar{h}_g)$

$$\frac{\partial \bar{C}_1}{\partial \bar{x}} = \beta_1 \frac{\partial^2 \bar{C}_1}{\partial \bar{y}^2} + \gamma_1 \frac{\partial^2 \bar{C}_1}{\partial \bar{z}^2} - \alpha_1 \bar{C}_1 \tag{7.22}$$

$$\bar{C}_1 = 0 \quad \text{at} \quad \bar{x} = 0 \tag{7.23}$$

$$\bar{C}_1 = 0 \quad \text{as} \quad \bar{y} \to \pm\infty \tag{7.24}$$

$$\frac{\partial \bar{C}_1}{\partial \bar{z}} = N_1 \bar{C}_1 \quad \text{at} \quad \bar{z} = 0 \tag{7.25}$$

$$\bar{K}_{z1} \frac{\partial \bar{C}_1}{\partial \bar{z}} = \bar{K}_{z2} \frac{\partial \bar{C}_2}{\partial \bar{z}}, \quad \bar{C}_1 = \bar{C}_2 \quad \text{at} \quad \bar{z} = \bar{h}_g \tag{7.26}$$

Region II $(\bar{h}_g \le \bar{z} \le 1)$

$$\frac{\partial \bar{C}_2}{\partial \bar{x}} = \beta_2 \frac{\partial \bar{C}_2}{\partial \bar{y}^2} + \gamma_2 \frac{\partial^2 \bar{C}_2}{\partial \bar{z}^2} - \alpha_2 \bar{C}_2 \tag{7.27}$$

$$\bar{C}_2 = \frac{1}{\bar{u}_2}\,\delta(\bar{y})\,\delta(\bar{z}-\bar{h}_s) \qquad \text{at } x = 0 \tag{7.28}$$

$$\bar{C}_2 = 0 \quad \text{as} \quad \bar{y} \to \pm\infty \tag{7.29}$$

$$\frac{\partial \bar{C}_2}{\partial \bar{z}} = 0 \quad \text{at} \quad \bar{z} = 1 \tag{7.30}$$

$$\bar{K}_{z2}\frac{\partial \bar{C}_2}{\partial \bar{z}} = \bar{K}_{z1}\frac{\partial \bar{C}_1}{\partial \bar{z}}\,, \quad \bar{C}_1 = \bar{C}_2 \text{ at } \bar{z} = \bar{h}_g \tag{7.31}$$

Region III ($0 \leq \bar{z} \leq \bar{h}_g$) $\bar{x} \geq \bar{x}_1$

$$\frac{\partial \bar{C}_3}{\partial \bar{x}} = \beta_3\frac{\partial^2 \bar{C}_3}{\partial \bar{y}^2} + \gamma_3\frac{\partial^2 \bar{C}_3}{\partial \bar{z}^2} - (\alpha_3+\lambda_3)\bar{C}_3 \tag{7.32}$$

$$\bar{C}_3 = \bar{C}_1 \quad \text{at} \quad \bar{x} = \bar{x}_1 \tag{7.33}$$

$$\bar{C}_3 = 0 \quad \text{as} \quad \bar{y} \to \pm\infty \tag{7.34}$$

$$\frac{\partial \bar{C}_3}{\partial \bar{z}} = N_2\bar{C}_3 \quad \text{at} \quad \bar{z} = 0 \tag{7.35}$$

$$\bar{K}_{z3}\frac{\partial \bar{C}_3}{\partial \bar{z}} = \bar{K}_{z4}\frac{\partial \bar{C}_4}{\partial \bar{z}}\,, \quad \bar{C}_3 = \bar{C}_4 \text{ at } \bar{z} = \bar{h}_g \tag{7.36}$$

Region IV ($\bar{h}_g \leq \bar{z} \leq 1$) $\bar{x} \geq \bar{x}_1$

$$\frac{\partial \bar{C}_4}{\partial \bar{x}} = \beta_4\frac{\partial^2 \bar{C}_4}{\partial \bar{y}^2} + \gamma_4\frac{\partial^2 \bar{C}_4}{\partial \bar{z}^2} - \alpha_4\bar{C}_4 \tag{7.37}$$

$$\bar{C}_4 = \bar{C}_2 \quad \text{at} \quad \bar{x} = \bar{x}_1 \tag{7.38}$$

$$\bar{C}_4 = 0 \quad \text{as} \quad \bar{y} \to \pm\infty \tag{7.39}$$

$$\frac{\partial \bar{C}_4}{\partial \bar{z}} = 0 \quad \text{at } \bar{z} = 1 \tag{7.40}$$

$$\bar{K}_{z4}\frac{\partial \bar{C}_4}{\partial \bar{z}} = \bar{K}_{z3}\frac{\partial \bar{C}_3}{\partial \bar{z}}, \ \bar{C}_4 = \bar{C}_3 \ \text{at} \ \bar{z} = \bar{h}_g \tag{7.41}$$

where

$$\beta_i = \frac{K_{yi}}{K_{zmax}\bar{u}_i}, \quad \gamma_i = \frac{\bar{K}_{zi}}{\bar{u}_i}$$

$$N_1 = \frac{\bar{v}_{d1}}{\bar{K}_{z2}}, \ N_2 = \frac{\bar{v}_{d2}}{\bar{K}_{z3}}, \ \alpha = \frac{kH^2}{K_{z\,max}}, \ \alpha_i = \frac{\alpha}{\bar{u}_i}$$

$$\lambda_3 = \frac{\bar{\lambda}}{\bar{u}_3}, \ \bar{\lambda} = \frac{\lambda H^2}{K_{zmax}}$$

The solutions $C_1\ (x,y,z)$, $C_2(x,y,z)$ of equations (7.22) and (7.27) subject to boundary conditions (7.23-7.26) and (7.28-7.31) have been obtained in Chapter VI.

Similarly, the solutions of equations (7.32) and (7.37) under the condition $\frac{K_{y3}}{u_3} = \frac{K_{y4}}{u_4}$, and subject to boundary conditions (7.33-7.36) and (7.38-7.41) are obtained as follows (dropping bars for convenience):

$$C_3(x,y,z) = \frac{e^{-\left(\frac{y^2}{4\beta'_3}\right)}}{\sqrt{4\pi\beta'_3}} \sum_{n=1}^{\infty} e^{-\delta'^2_n (x-x_1)} R'_n\, G_{1n}(z) \tag{7.42}$$

$$C_4(x,y,z) = \frac{e^{-\left(\frac{y^2}{4\beta'_3}\right)}}{\sqrt{4\pi\beta'_3}} \sum_{n=1}^{\infty} e^{-\delta'^2_n (x-x_1)} R'_n\, G_{2n}(z) \tag{7.43}$$

where,

$$R'_n = \frac{\int_0^{h_g} u_3 C_1(x,z) G_{1n}(z)\,dz + \int_{h_g}^{1} u_4 C_2(x,z) G_{2n}(z)\,dz}{\int_0^{h_g} u_3\, G_{1n}^2(z)\,dz + \int_{h_g}^{1} u_4\, G_{2n}^2(z)\,dz} \tag{7.44}$$

$$G_{1n}(z) = \frac{\left(\frac{N_2}{a'_{11}} \sin a'_{11}z + \cos a'_{11}z\right)}{\left(\frac{N_2}{a'_{11}} \sin a'_{11} h_g + \cos a'_{11}h_g\right)}$$

$$G_{2n}(z) = \frac{(\tan a'_{12} \sin a'_{12}z + \cos a'_{12}z)}{(\tan a'_{12} \sin a'_{12} h_g + \cos a'_{12}h_g)}$$

$$\beta'_3 = \beta_3(x-x_1) + \beta_1 x_1$$

$$a'_{11} = \sqrt{(\delta'^{\,2}_n - \alpha_3 - \lambda_3)/\gamma_3} \qquad a'_{12} = \sqrt{(\delta'^{\,2}_n - \alpha_3)/\gamma_4}$$

and δ'_ns are eigen values of following equation

$$K_{z3} \frac{(N_2 \cos a'_{11} h_g - a'_{11} \sin a'_{11} h_g)}{\left(\frac{N_2}{a'_{11}} \sin a'_{11} h_g + \cos a'_{11} h_g\right)} =$$

$$K_{z4} \frac{(a'_{12} \tan a'_{12} \cos a'_{12} h_g - a'_{12} \sin a'_{12} h_g)}{(\tan a'_{12} \sin a'_{12} h_g + \cos a'_{12} h_g)} \tag{7.45}$$

When the source lies in the second region, the concentration distributions $C_1(x,z)$, $C_2(x,z)$ involved in equation (7.44) are given by equations (6.39) and (6.40) in Chapter VI.

Similarly when source lies in the first region, corresponding $C_1(x,z)$, $C_2(x,z)$ are given by equations (6.41) and (6.42) in Chapter VI.

(ii) DISPERSION FROM A LINE SOURCE

In this case, the concentration distributions $C_1(x,z)$, $C_2(x,z)$ corresponding to region I and II have been obtained in Chapter VI and are given by equations (6.39) and (6.40). For the region III, IV, the concentration distributions are obtained by integrating equations (7.42-7.43) between $-\infty$ to ∞ with respect to y and written as follows.

$$C_3(x,z) = \sum_{n=1}^{\infty} e^{-\delta_n'^2 (x-x_1)} R_n' G_{1n}(z) \tag{7.46}$$

$$C_4(x,z) = \sum_{n=1}^{\infty} e^{-\delta_n'^2 (x-x_1)} R_n' G_{2n}(z) \tag{7.47}$$

where R_n' is defined by equation (7.44).

7.3 RESULTS AND DISCUSSION

To study the depletion of pollutant due to green-belt, the following values of parameters have been chosen for computation: $u_1 = 0.55$, $u_2 = 1.0$, $u_3 = 0.5$, $u_4 = 1.0$, $H = 200$m $K_{z1} = 0.55$, $K_{z2} = 1.0$, $K_{z3} = 0.5$, $K_{z4} = 1.0$, $\beta_1 = \beta_2 = \beta_3 = \beta_4 = 10$, $\alpha = 0.11$, $\lambda = 4.0$ and $h_g = .05$. By taking various heights of source, the vertical concentration distributions

of pollutant havebeen computed at the end of green belt and depicted in figs. 7.2-7.4 It is noted that the concentration of pollutant decreases in the presence of green belt.

If we compare figs. 7.3 and 7.4 it is found that the depletion in the concentration of pollutant due to green belt is greater if the height of source is less than the height of green belt.

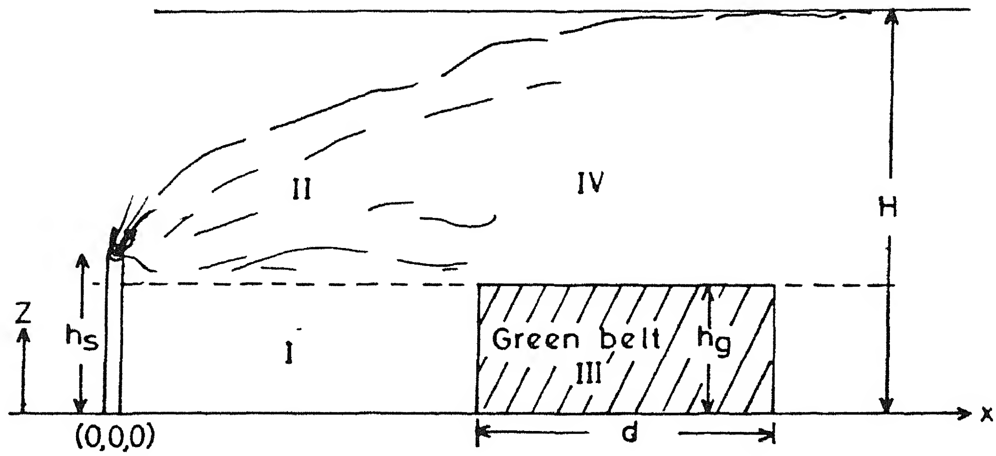

FIG 7.1

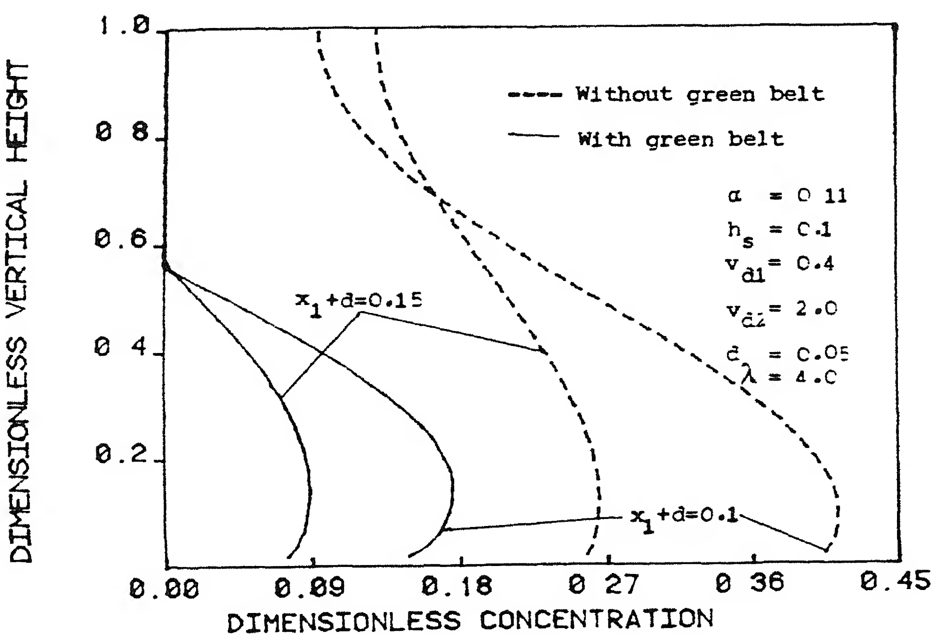

FIG 7.2 VERTICAL CONCENTRATION PROFILE WHEN $h_s > h_g$

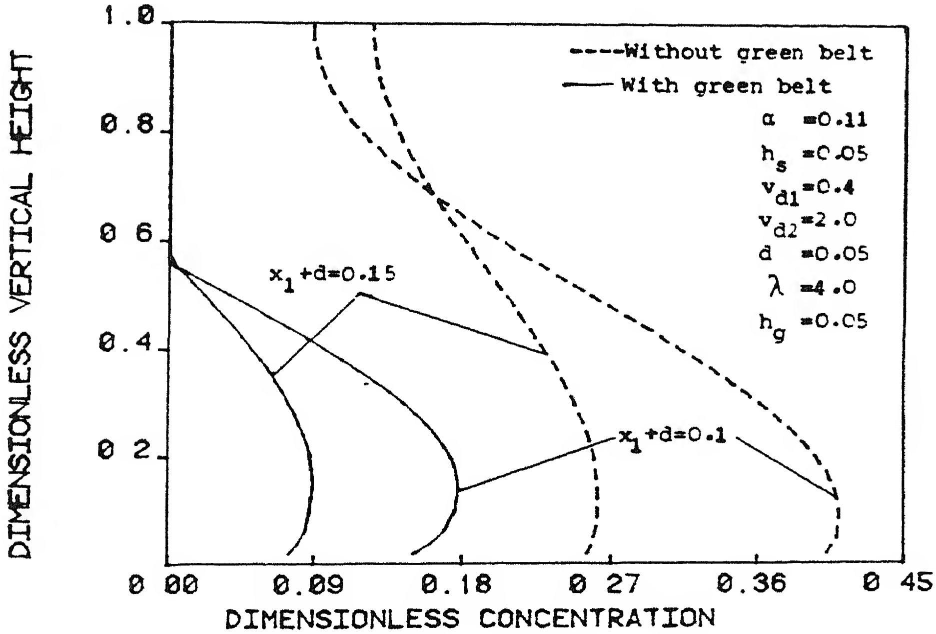

FIG 7.3 VERTICAL CONCENTRATION PROFILE WHEN $h_s = h_g$

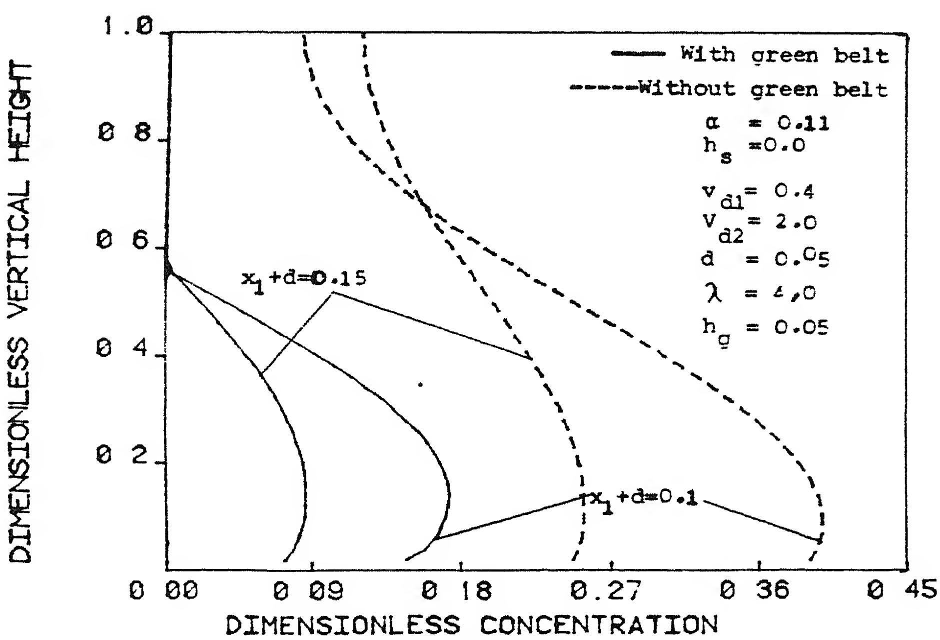

FIG 7 4 VERTICAL CONCENTRATION PROFILE WHEN $h_s < h_g$

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CHAPTER VIII

UNSTEADY STATE DISPERSION OF A REACTIVE AIR POLLUTANT : EFFECT OF GREEN BELT

8.1 INTRODUCTION

The effect of removal on the steady state dispersion of a reactive air pollutant due to presence of green belt has been discussed in Chapter VII. In this chapter, the same problem is investigated for unsteady state dispersion of a reactive pollutant in the atmosphere emitted from a point source. It is assumed that the green belt lies away from the source in the wind direction and is acting as a sink so that the pollutant can be removed by chemical reaction, deposition absorption, etc. In the region of green belt, we consider the unsteady state diffusion equation with a removal term proportional to the concentration of pollutant such that the magnitude of removal rate coefficient depend on the number and size of plants in the green belt (Slinn, 1982; Wiman and Agren (1985)). However, in the region without green belt; the usual unsteady state diffusion equation with chemical reaction is taken.

8.2 MATHEMATICAL FORMULATION AND SOLUTIONS

Consider the unsteady state dispersion of a reactive pollutant from a time dependent point source in presence of gree

belt under the inversion condition. Assume that the green bel· of thickness d is located at a distance x_1 from the source in the wind direction. The region under consideration $0 \leq x \leq x_1 + d$ is divided into two parts, the green belt is assumed to exist in the second region. It is assumed that the wind speed is sufficient large in both the regionsso that diffusion in x-direction can be neglected in comparison to advection. In writing the mathematical model it is considered that the green belt is equivalent to point sinks distributed all over the second region. Thus, the partial differential equations governing the concentration of pollutant in the two regions car be written as follows :

Region I $\quad x \leq x_1$

$$\frac{\partial C_1}{\partial t} + u_1 \frac{\partial C_1}{\partial x} = K_{y1} \frac{\partial^2 C_1}{\partial y^2} + K_{z1} \frac{\partial^2 C_1}{\partial z^2} - k\, C_1 \tag{8.1}$$

with boundary conditions

$$C_1 = 0 \quad \text{at } t = 0 \tag{8.2}$$

$$C_1 = \frac{W(t)}{u_1} \delta(y)\, \delta(z-h_s) \quad \text{at } x = 0 \tag{8.3}$$

$$C_1 = 0 \quad \text{as} \quad y \to \pm \infty \tag{8.4}$$

$$\frac{\partial C_1}{\partial z} = 0 \quad \text{at} \quad z = H \tag{8.5}$$

$$K_{z1} \frac{\partial C_1}{\partial z} = v_{d1}\, C_1 \quad \text{at } z = 0 \tag{8.6}$$

Region II $x \geq x_1$

$$\frac{\partial C_a}{\partial t} + u_a \frac{\partial C_a}{\partial x} = K_{ya} \frac{\partial^2 C_a}{\partial y^2} + K_{za} \frac{\partial^2 C_a}{\partial z^2} - (k + \lambda)C_a \tag{8.7}$$

and boundary conditions are

$$C_a = 0 \qquad \text{at } t = 0 \tag{8.8}$$

$$C_a = C_1 \qquad \text{at } x = x_1 \tag{8.9}$$

$$C_a = 0 \qquad \text{as } y \rightarrow \pm \infty \tag{8.10}$$

$$\frac{\partial C_a}{\partial z} = 0 \qquad \text{at } z = H \tag{8.11}$$

$$K_{za} \frac{\partial C_a}{\partial z} = v_{d2} C_a \text{ at } z = 0 \tag{8.12}$$

where C_1, C_a are concentrations of pollutant in each region, u_1, u_a are mean wind velocities, K_{y1}, K_{ya} and K_{z1}, K_{za} are diffusion coefficients in y- and z-directions respectively. v_{d1}, v_{d2} are dry deposition velocity on the ground in the different regions. k is chemical reaction rate, λ is the deplection rate of pollutan due to green belt.

As in Chapter IV, the following forms of W(t) would be considered in the subsequent analysis :

(i) Flux is instantaneous

$W(t) = W_o \, \delta(t)$

(ii) Flux is constant

$W(t) = W_c$ (constant) (8.13)

(iii) Flux is step function type

$$W(t) = W_c \qquad 0 \le t \le t_o$$
$$\quad = 0 \qquad\qquad t > t_o$$

The concentration distribution of pollutant for region I is

(i) For instantaneous case

$$C_1(x,y,z,t) = \frac{W_o}{u_1} P(x,y,z)\ \delta(t - \frac{x}{u_1}) \tag{8.14}$$

(ii) For constant case

$$C_1(x,y,z,t) = \frac{W_c}{u_1} P(x,y,z)\ H(t - \frac{x}{u_1}) \tag{8.15}$$

(iii) For step function type flux

$$C_1(x,y,z,t) = \frac{W_c}{u_1} P(x,y,z)\ [H(t - \frac{x}{u_1}) - H(t - \frac{x}{u_1} - t_o)\ H(t-t_o)] \tag{8.16}$$

where

$$P(x,y,z) = \frac{\exp\left(\dfrac{-y^2}{4\dfrac{K_{y1}}{u_1}x}\right)}{\sqrt{4\pi \dfrac{K_{y1}}{u_1} x}} \sum_{n=1}^{\infty} \frac{1}{P_n} \cos \lambda_n (z-H)$$

$$\times \cos \lambda_n (h_s - H)\, e^{-\left(\frac{k}{u_1} + \frac{K_{z1}}{u_1}\lambda_n^2\right)x}$$

$$P_n = \int_0^H \cos^2 \lambda_n (z-H) dz$$

and λ_n's are solutions of following transcendental equation

$$\lambda_n \tan \lambda_n H = \frac{v_{d1}}{K_{z1}} \tag{8.17}$$

The concentration distribution of pollutant in second region is obtained as :

(i) Flux is instantaneous

$$C_a = \frac{W_o}{u_1} M(x,y,z)\ \delta\left(t - \left(\frac{x_1}{u_1} + \frac{x-x_1}{u_a}\right)\right) \tag{8.18}$$

(ii) Flux is constant

$$C_a = \frac{W_c}{u_1} M(x,y,z)\ H\left(t - \left(\frac{x_1}{u_1} + \frac{x-x_1}{u_a}\right)\right) \tag{8.19}$$

(iii) Flux is step function type

$$C_a = \frac{W_c}{u_1} M(x,y,z)\ \left[H\left(t-\left(\frac{x_1}{u_1} + \frac{x-x_1}{u_a}\right)\right) - H\left(t-t_o-\left(\frac{x_1}{u_1} + \frac{x-x_1}{u_a}\right)\right) H(t-t_o)\right] \tag{8.20}$$

where

$$M(x,y,z) = \frac{\exp\left(-\frac{y^2}{4\beta(x)}\right)}{\sqrt{4\pi\ \beta(x)}} \sum_{n=1}^{\infty} \frac{\cos \mu_n (z-H)}{Q_n}$$

$$\times \exp\left[-k\left(\frac{x_1}{u_1} + \frac{x-x_1}{u_a}\right) - \frac{\lambda}{u_a}(x-x_1) - \frac{K_{z1}}{u_a}\mu_n^2 (x-x_1)\right]$$

$$\times \sum_{m=1}^{\infty} \frac{1}{P_m} \cos \lambda_m (h_s - H) \exp\left[-\frac{K_{z1}}{u_1}\lambda_m^2\ x_1\right]$$

$$\times \int_0^H \cos \lambda_m (z-H) \cos \mu_n (z-H)\ dz$$

$$Q_n = \int_0^H \cos^2 \mu_n (z-H)\ dz,$$

μ_n's are roots of following equation

$$\mu_n \tan \mu_n H = \frac{v_{d2}}{K_{za}}$$

and

$$\beta(x) = \frac{K_{y1} x_1}{u_1} + \frac{K_{ya}}{u_a} (x - x_1).$$

Using the following dimensionless quantities

$$\bar{x} = \frac{K_{z\,max}\, x}{u_{max}\, H^2}, \quad \bar{y} = \frac{y}{H}, \quad \bar{z} = \frac{z}{H}, \quad \bar{u}_1 = \frac{u_1}{u_{max}}, \quad \bar{u}_a = \frac{u_a}{u_{max}}$$

$$\bar{K}_{z1} = \frac{K_{z1}}{K_{z\,max}}, \quad \bar{K}_{za} = \frac{K_{za}}{K_{z\,max}}, \quad \bar{v}_{di} = \frac{v_{di}\, H}{K_{z\,max}}, \quad \bar{t} = \frac{K_{z\,max}\, t}{H^2}$$

$$\bar{C}_1 = \frac{u_{max}\, H^2 C_1}{W_c}, \quad \bar{C}_a = \frac{u_{max}\, H^2 C_a}{W_c}, \quad \bar{k} = \frac{k\, H^2}{K_{z\,max}},$$

$$\bar{\lambda} = \frac{\lambda H^2}{K_{z\,max}}, \quad \bar{W}_o = \frac{W_o\, H^2}{W_c\, K_{z\,max}}, \quad \bar{W}(t) = \frac{W(t)}{W_c}$$

$$\bar{h}_s = \frac{h_s}{H}, \quad \bar{\lambda}_n = \lambda_n H, \quad \bar{\mu}_n = \mu_n H, \quad (i=1,2;\ n=1,2,\ldots) \tag{8.21}$$

the concentration distribution of pollutant given by equations (8.14 - 8.16) can be transformed in dimensionless form (dropping bars for convenience) as,

Region I $\quad x \leq x_1$

(i) Flux is instantaneous

$$C_1(x,y,z,t) = \frac{W_o}{u_1} P(x,y,z)\, \delta\left(t - \frac{x}{u_1}\right) \tag{8.22}$$

(ii) Flux is constant,

$$C_1(x,y,z,t) = \frac{1}{u_1} P(x,y,z)\, H\left(t - \frac{x}{u_1}\right) \tag{8.23}$$

(iii) Flux is step function type

$$C_1(x,y,z,t) = \frac{P(x,y,z)}{u_1}\left[H(t-\frac{x}{u_1}) - H(t-t_o - \frac{x}{u_1})H(t-t_o)\right] \tag{8.24}$$

where

$$P(x,y,z) = \frac{\exp\left(\dfrac{-y^2}{4\dfrac{K_{y1}}{K_{z\,max}\,u_1}x}\right)}{\sqrt{4\pi\dfrac{K_{y1}}{K_{z\,max}\,u_1}x}} \sum_{n=1}^{\infty} \frac{1}{P_n} \cos\lambda_n(z-1)$$

$$\times \cos\lambda_n(h_s-1)\; e^{-(\frac{k}{u_1} + \frac{K_{z1}}{u_1}\lambda_n^2)x} \tag{8.25}$$

$$P_n = \int_0^1 \cos^2\lambda_n(z-1)\,dz$$

and λ_n's are roots of following transcendental equation

$$\lambda_n \tan\lambda_n = N_1'$$

$$N_1' = \frac{v_{d1}}{K_{z1}}.$$

Region II $\quad x \geq x_1$

(i) Flux is instantaneous

$$C_a = \frac{W_o}{u_1} M(x,y,z)\,\delta(t - (\frac{x_1}{u_1} + \frac{x-x_1}{u_a})) \tag{8.26}$$

(ii) Flux is constant

$$C_a = u_1\, M(x,y,z)\, H(t - (\frac{x_1}{u_1} + \frac{x-x_1}{u_a})) \tag{8.27}$$

(iii) Flux is step function type

$$C_a = \frac{M(x,y,z)}{u_1} \left[H(t - (\frac{x_1}{u_1} + \frac{x-x_1}{u_a})) - H(t-t_o - (\frac{x_1}{u_1} + \frac{x-x_1}{u_a})) H(t-t_o \right. \quad (8.28)$$

where

$$M(x,y,z) = \frac{\exp(-\frac{y^2}{4\beta(x)})}{\sqrt{4\pi\ \beta(x)}} \sum_{n=1}^{\infty} \frac{\cos \mu_n (z-1)}{Q_n}$$

$$\times \exp\left[-k(\frac{x_1}{u_1} + \frac{x-x_1}{u_a}) - \frac{\lambda}{u_a}(x-x_1) - \frac{K_{z1}}{u_a} \mu_n^2 (x-x_1)\right]$$

$$\times \sum_{m=1}^{\infty} \frac{1}{P_m} \cos \lambda_m (h_s - 1) \exp\left[-\frac{K_{z1}}{u_1} \lambda_m^2\ x_1\right]$$

$$\times \int_0^1 \cos \lambda_m (z-1) \cos \mu_n (z-1)\ dz \quad (8.29)$$

$$Q_n = \int_0^1 \cos^2 \mu_n (z-1)\ dz$$

$$\beta(x) = \beta_1 x_1 + \beta_a (x-x_1)$$

$$\beta_1 = \frac{K_{y1}}{K_{z\ max}\ u_1}, \quad \beta_a = \frac{K_{ya}}{K_{z\ max}\ u_a}$$

$$K_{z\ max} = \max(K_{z1}, K_{za})$$

$$u_{max} = \max(u_1, u_a)$$

and μ_n's are roots of following equation

$$\mu_n \tan \mu_n = \frac{v_{d2}}{K_{za}}$$

STEADY STATE CASE

In such a case $t \to \infty$, the corresponding expressions for concentration distributions in the two regions can be obtaine from equations (8.23) and (8.27) as follows (in the case of continuous point source) :

$$C_1 = \frac{1}{u_1} P(x,y,z)$$

$$C_a = \frac{1}{u_1} M(x,y,z)$$

where $P(x,y,z)$ and $M(x,y,z)$ are defined in previous section [see equations (8.25), (8.29)] . It is remarkable that these expressions can also be obtained from equations (6.39 - 6.40) in Chapter VI assuming $u_1 = u_2$, $K_{z1} = K_{z2}$, $K_{y1} = K_{y2}$ and by taking $u_3 = u_4 = u_a$, $K_{z3} = K_{z4} = K_{za}$, $K_{y3} = K_{y4} = K_{ya}$ in equations (7.42 - 7.43) in Chapter VII.

8.3 RESULTS AND DISCUSSION

For unsteady case, the concentration distributions of pollutant for different values of t, $u_1 = u_a = 1.0$, $K_{z1} = K_{za}=1.$ $\beta_1 = \beta_a = 10.0$, $\alpha = 0.11$, $\lambda = 5.0$, are computed and shown in figs. (8.1,8.2,8.3). It is seen from these graphs that the concentration of pollutant decreases in the region of green belt in all the three cases. The vertical concentration profile of pollutant is depicted in fig. (8.4) for $\lambda = 6.0$, 10.0, $u_1 = 1.0$, $u_a = 1.0$, $K_{z1} = 1.0$, $K_{za} = 1.0$, $\alpha = 0.11$ and $\beta_1 = 10.0$, $\beta_a = 10.$ and $x_2 = 0.1$ (end of the green belt). It is observed that the

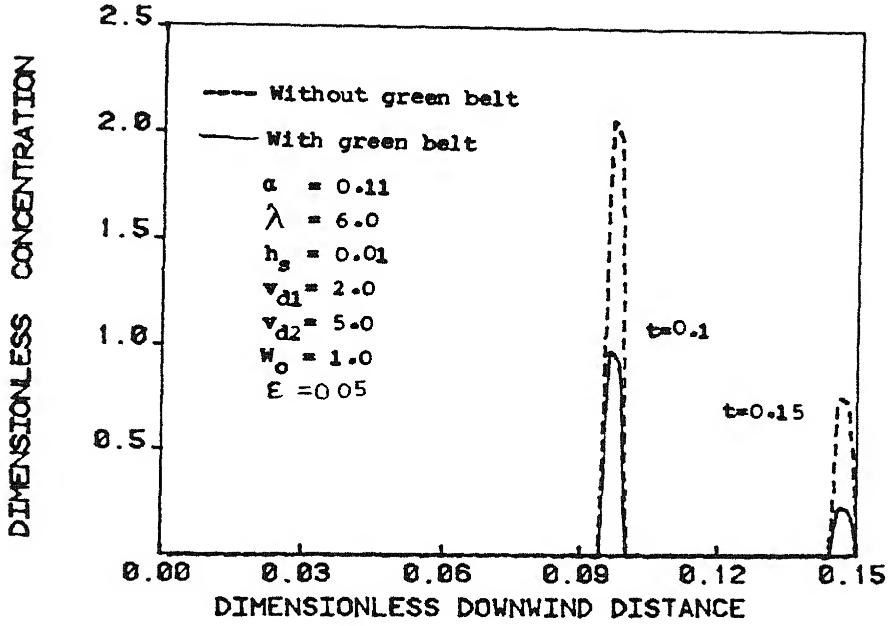

FIG 8 1 FLUX IS INSTANTANEOUS AT THE SOURCE

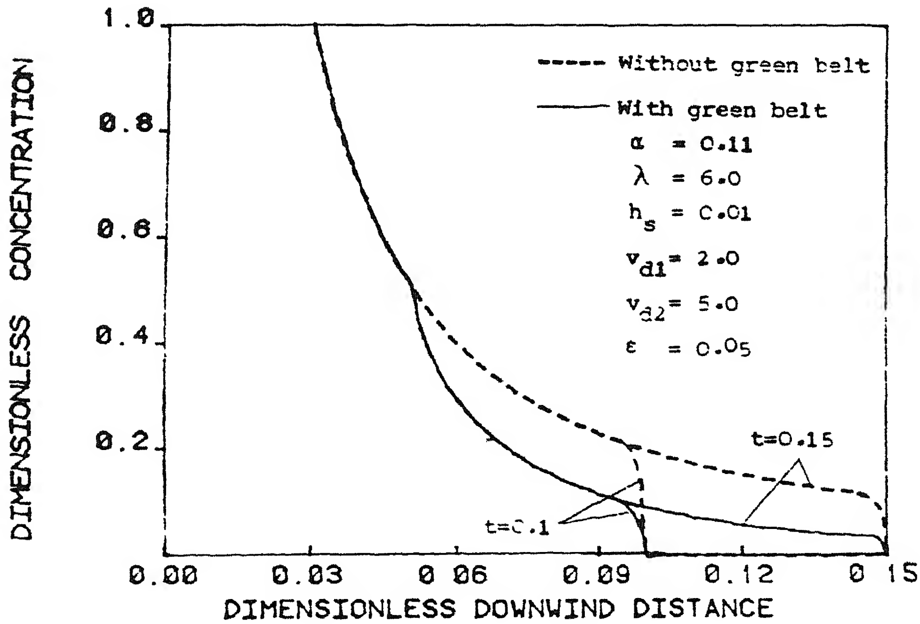

FIG 8.2 FLUX IS CONSTANT AT THE SOURCE

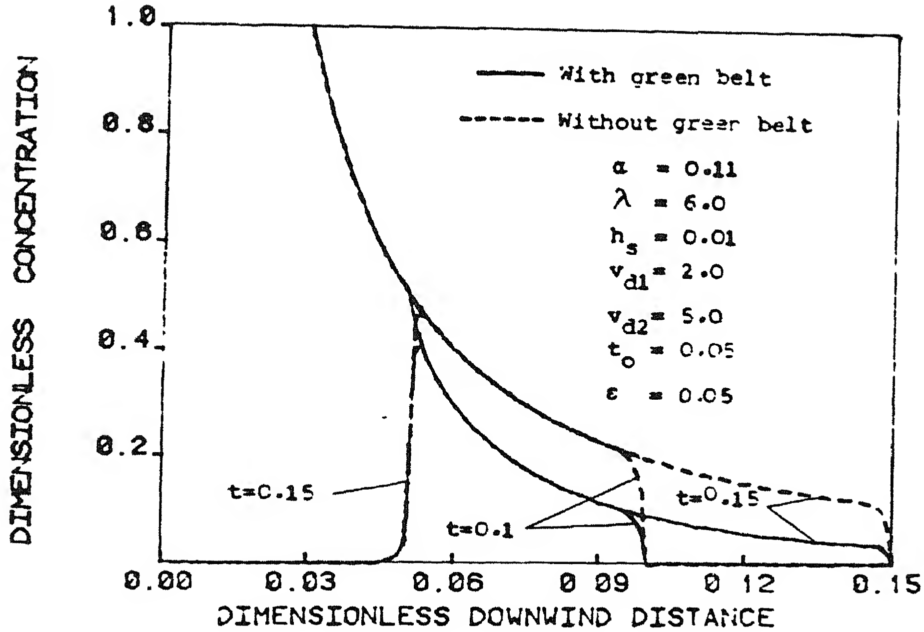

FIG 8.3 FLUX IS STEP FUNCTION TYPE AT THE SOURCE

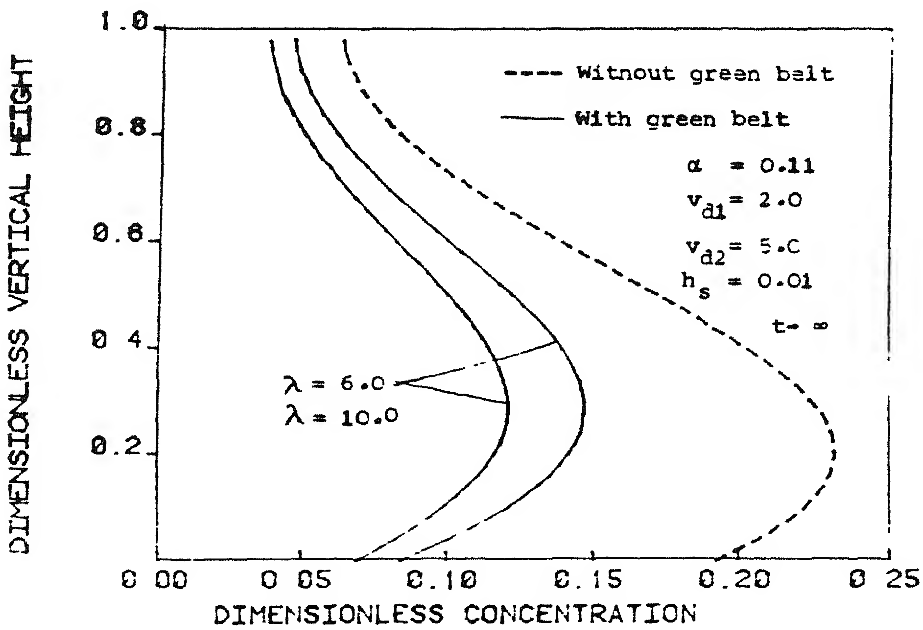

FIG 8 4 EFFECT OF λ ON THE CONCENTRATION OF POLLUTANT

concentration of pollutant decreases as λ increases.

The analysis presented in this chapter shows the importance of green belt in reducing the concentration of air pollutant emitted from time dependent sources such as accidental leakage of gases etc. and there by protecting region under consideration.

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CHAPTER IX

ATMOSPHERIC DISPERSION MODEL WITH INTEGRAL TERM FOR REMOVAL MECHANISM*

9.1 INTRODUCTION

The study of atmospheric dispersion of air pollutants from point source, line and area has received a great deal of attention during last few decades (Smith, 1957; Pasquill, 1962; Gifford and Hanna, 1971, Heines and Peters, 1973a, 1973b; Lebedeff and Hameed, 1975; Ragland, 1973; Ermak, 1977; Dobbins, 1979; Karamchandani and Peters, 1983). Effects of removal process on the dispersal of air pollutants have also been investigated (Scriven and Fisher, 1975a, 1975b; Alam and Seinfeld, 1981, Fisher, 1982, Llewelyn, 1983). When air pollutants are removed by rainout/washout in the environment the dispersal process becomes very complex and very little attention has been given to understand this mechanism (Hales, 1972; Slinn, 1974; Alam and Seinfeld, 1981).

In view of this, in this chapter a growth equation is suggested to study the removal of air pollutant by rain or fog droplets. In such a case the unsteady state partial differential equation for dispersion of air pollutant is modified into the form of an integro-differential equation.

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To explain the effect of removal process by this model, we have studied the dispersion of air pollutant from an elevated time dependent point source which may be applicable during mansoon season in India.

9.2 MATHEMATICAL FORMULATION

Consider the dispersion of air pollutant from an elevated time-dependent point source in a stable environment such that the wind velocity may be assumed to be uniform. In such a case, the three dimensional transport equation in cartesian coordinates (x,y,z) for air pollutant concentration C is written in the following form

$$\frac{\partial C}{\partial t} + U\frac{\partial C}{\partial x} = D\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2}\right) - kC \qquad (9.1)$$

where U is mean wind velocity, D is diffusion coefficient assumed to be constant and k is the removal rate.

When the fog or rain droplets are present in the environment, the air pollutant gets absorbed in the droplet phase and this removal process is not instantaneous. Assuming that the rate of decrease of pollutant (i.e. $\frac{\partial C}{\partial t}$) is proportional to its concentration C_r in the droplet phase, the transport equation (9.1) in this case may be modified as

$$\frac{\partial C}{\partial t} + U\frac{\partial C}{\partial x} = D\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2}\right) - k_o C_r(x,y,z,t) \qquad (9.2)$$

Since the rate of change of the concentration of air pollutant in the droplet phase (i.e. $\frac{\partial C_r}{\partial t}$) may increase with the increase of concentration of pollutant C and decrease due to rainout/washout, the governing equation for C_r can be written as,

$$\frac{\partial C_r}{\partial t} = \alpha_o C - \alpha C_r \tag{9.3}$$

where α_o, α are constant rates of absorption and removal. Now integrating equation (9.3) with the condition $C_r = 0$ at $t = 0$, we get

$$C_r(x,y,z,t) = \alpha_o \int_o^t e^{-\alpha(t-T)} C(x,y,z,T)\, dT \tag{9.4}$$

Equation (9.2) then becomes

$$\frac{\partial C}{\partial t} + U\frac{\partial C}{\partial x} = D\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2}\right) - \alpha_1 \int_o^t e^{-\alpha(t-T)} C(x,y,z,T)\, dT \tag{9.5}$$

where the integral term represents the removal of air pollutant by the droplet phase and $\alpha_1 = \alpha_o k_o$.

It may be noted here that equations (9.1) and (9.5) can be combined as follows:

$$\frac{\partial C}{\partial t} + U\frac{\partial C}{\partial x} = D\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2}\right) - \int_o^t G(t-T)\, C(x,y,z,T)\, dT \tag{9.6}$$

where for $G(t-T) = k\delta(t-T)$, $\delta(.)$ is Dirac delta function, the equation (9.6) reduces to (9.1) and for $G = \alpha_1 e^{-\alpha(t-T)}$, we get equation (9.5).

Thus, equation (9.6) may be interpreted as a general transport diffusion equation with an integral term representing the removal mechanism. Equation (9.1) may be designated as diffusion equation with instantaneous removal term while equation (9.5) may represent the case with delayed (slow) removal process.

It is noted here that under steady state condition equation (9.3) gives $C_r = \frac{\alpha_o k_o}{\alpha} C$. In such case, equations (9.1) and (9.2) would become identical provided $k = \frac{\alpha_o k_o}{\alpha} = \frac{\alpha_1}{\alpha}$ and two removal mechanisms would be same under this condition. However, under unsteady condition these removal mechanisms are different.

In the following, therefore, we study the dispersion of air pollutant with delayed and instantaneous removal processes under the condition when k is greater, less or equal to $\frac{\alpha_1}{\alpha}$.

The initial and boundary conditions for (9.1) and (9.5), taking the source as the origin of coordinate system, are written as

$$C(s,t) = 0 \text{ at } t = 0 \text{ for all } s = \sqrt{x^2+y^2+z^2} > 0 \tag{9.7}$$

$$C(s,t) = 0 \text{ as } s \to \infty \text{ for } t \geq 0 \tag{9.8}$$

$$-4\pi s^2 D \frac{\partial C}{\partial s} = W(t) \text{ as } s \to 0 \text{ for } t \geq 0. \tag{9.9}$$

The last boundary condition implies that the point source

has prescribed time dependent flux. In this chapter, the following forms of $W(t)$ are considered.

$$
\begin{aligned}
&\text{(i)} \quad W(t) = W_o \delta(t) \\
&\text{(ii)} \quad W(t) = W_c \\
&\text{(iii)} \quad W(t) = W_c \quad 0 \le t \le t_o \\
&\qquad\qquad\quad = 0 \quad t > t_o
\end{aligned}
\tag{9.10}
$$

where $\delta(.)$ is Dirac delta function.

Define the following dimensionless quantities

$$
\begin{aligned}
&\bar{t} = \frac{u^{*2}}{D} t, \quad \bar{U} = \frac{U}{u^*}, \quad \bar{\alpha}_1 = \frac{D^2}{u^{*4}} \alpha_1 \\
&\bar{\alpha} = \frac{D}{u^{*2}} \alpha, \quad \bar{s} = \frac{u^*}{D} s, \quad \bar{x} = \frac{u^*}{D} x, \bar{y} = \frac{u^*}{D} y \\
&\bar{z} = \frac{u^*}{D} z, \quad \bar{k} = \frac{kD}{u^{*2}}, \quad \bar{C} = \frac{u^* W_c}{D^2} C.
\end{aligned}
\tag{9.11}
$$

where u^* is friction velocity.

Using above dimensionless quantities equations (9.5-9.10) can be written in dimensionless form (dropping bars for convenience) as

$$
\frac{\partial C}{\partial t} + U \frac{\partial C}{\partial x} = \frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2} - \alpha_1 \int_0^t e^{-\alpha(t-T)} C(x,y,z,T)\, dT
\tag{9.12}
$$

$$
C(s,t) = 0 \quad \text{at} \quad t = 0,\ s > 0 \tag{9.13}
$$

$$
C(s,t) = 0 \quad \text{as} \quad s \to \infty \quad t \ge 0 \tag{9.14}
$$

$$-4\pi s^2 \frac{\partial C}{\partial s} = \frac{W(t)}{W_c} \quad \text{as } s \to 0 \quad t \geq 0 \tag{9.15}$$

(i) $\frac{W(t)}{W_c} = Q_o \delta(t)$

(ii) $\frac{W(t)}{W_c} = 1$ (9.16)

(iii) $\frac{W(t)}{W_c} = 1 \qquad 0 \leq t \leq t_o$

$\qquad = 0 \qquad t > t_o$

where

$$Q_o = \frac{W_o D}{u^{*2} W_c}.$$

9.3 METHOD OF SOLUTION

Taking Laplace transform of (9.12) and using initial condition (9.13), we get

$$u \frac{\partial \bar{C}}{\partial x} = \frac{\partial^2 \bar{C}}{\partial x^2} + \frac{\partial^2 \bar{C}}{\partial y^2} + \frac{\partial^2 \bar{C}}{\partial z^2} - m\bar{C} \tag{9.17}$$

where $\bar{C}$ is Laplace transform of C, $m = p + \frac{\alpha_1}{p+\alpha}$ and p is Laplace variable.

The boundary conditions become

$$\bar{C}(s,p) = 0 \quad s \to \infty$$

$$-4\pi s^2 \frac{\partial \bar{C}}{\partial s} = \frac{W(p)}{W_c} \quad s \to 0. \tag{9.18}$$

Assuming the solution of equation (9.17) of the form

$$\bar{C} = \exp\left(\frac{Ux}{2}\right) f(s,p)$$

and using (9.18), we get

$$\bar{C} = \frac{W(p)}{4\pi s W_c} \exp\left[\frac{Ux}{2} - \left(\frac{U^2}{4} + m\right)^{1/2} s \right] \tag{9.19}$$

Taking inverse Laplace transform of equation (9.19), the solution of (9.12) satisfying the initial and boundary conditions can be written as follows

$$C(x,y,z,t) = \frac{1}{4\pi s} \left(\frac{1}{2\pi i}\right) \int_{\gamma-i\infty}^{\gamma+i\infty} \frac{W(p)}{W_c} \exp\left[pt + \frac{Ux}{2} - \left\{\frac{(p+a)(p+a')}{(p+\alpha)}\right\}^{1/2} s\right] dp \tag{9.20}$$

where

$(a,a') = \frac{1}{2}\left(\frac{U^2}{4} + \alpha\right) \mp \left\{\left(\frac{U^2}{4} - \alpha\right)^2 - 4\alpha_1\right\}^{1/2}$ and γ is a real positive number such that all the singularities of the integrand lie on the left handside of line $Re(p) = \gamma$ in the Bromwich contour (Carslaw and Jaeger, 1959). The integral in equation (9.20) can be evaluated and the concentration along the central line for each case can be found as follows.

(i) when the flux is instantaneous, i.e. $W(t) = W_o \delta(t)$

$$C(x,0,0,t) = \frac{Q_o P(x)}{4\pi^2 x} \int_a^{\alpha} M(x,u,t)\,du + \int_{a'}^{\infty} M(x,u,t)\,du \tag{2.21}$$

where $P(x) = \exp(Ux/2)$,

$$M(x,u,t) = e^{-ut} \sin \left[\frac{(u-a)(u-a')}{(u-\alpha)}\right]^{1/2} x.$$

Similarly the solution of equation (9.1) is obtained and the concentration along the central line in the dimensionless form is written as

$$C_1(x,0,0,t) = \frac{Q_o}{(4\pi t)^{3/2}} \exp\left[\frac{Ux}{2} - \left(\frac{U^2}{4} + k\right)t - \frac{x^2}{4t}\right] \qquad (9.22)$$

when $U = 0$ and $k = 0$, it is reduced to same form as the one obtained by Carslaw and Jaegar (1941).

(ii) When the flux is constant, i.e. $W(t) = W_c$

$$C(x,0,0,t) = \frac{P(x)}{4\pi x} \{\exp\left[-\left(\frac{U^2}{4} + \frac{\alpha_1}{\alpha}\right)^{1/2} x\right]\}$$

$$- \frac{1}{\pi} \int_a^{\alpha} \frac{1}{u} M(x,u,t)\,du$$

$$- \frac{1}{\pi} \int_{a'}^{\infty} \frac{1}{u} M(x,u,t)\,du\} \qquad (9.23)$$

From the above expression it is observed that the concentration of pollutant as $t \to \infty$ reaches to steady state, given by the following expression

$$C(x,0,0,t) = \frac{P(x)}{4\pi x} \{\exp\left[-\left(\frac{U^2}{4} + \frac{\alpha_1}{\alpha}\right)^{1/2} x\right]$$

Similarly solving equation (9.1) in this case the concentration distribution along the central line in the dimensionless form, is given by

$$C_1(x,0,0,t) = \frac{P(x)}{4\pi x} \{\exp\left[-\left(\frac{U^2}{4} + k\right)^{1/2} x\right]$$

$$- \frac{1}{\pi} \int_{a_1}^{\infty} \frac{1}{u} \exp(-ut) \sin(u-a_1)^{1/2} x\,du\} \qquad (9.24)$$

where

$$a_1 = \frac{U^2}{4} + k.$$

(iii) When the flux is step function i.e. $W(t) = W_o \quad 0 < t \le t_o$

$= 0 \quad t > t_o$

$$C(x,0,0,t) = \frac{P(x)}{4\pi x} \{\exp\left[-(\frac{U^2}{4} + \frac{\alpha_1}{\alpha})^{1/2} x\right] (1-H(t-t_o))$$

$$- \frac{1}{\pi} \int_a^{\alpha} \frac{1}{u} [1-e^{ut_o} H(t-t_o)] M(x,u,t)\, du$$

$$- \frac{1}{\pi} \int_{a'}^{\infty} \frac{1}{u} [1-e^{ut_o} H(t-t_o)] M(x,u,t)\, du\} \qquad (9.25)$$

Where $H(t-t_o)$ is defined by (Carslaw and Jaegar, 1941)

$$H(t-t_o) = 0 \qquad t \le t_o$$

$$= \frac{t}{t_o+\epsilon} \qquad t_o < t \le t_o + \epsilon$$

$$= 1 \qquad t > t_o.$$

In this case, for instantaneous removal the concentration distribution along the central line, in the diemsnsic.nless form, is given by

$$C_1(x,0,0,t) = \frac{P(x)}{4\pi x} \{\exp\left[-(\frac{U^2}{4} + k)^{1/2} x\right] \times$$

$$[1-H(t-t_o)] - \frac{1}{\pi} \int_{a_1}^{\infty} \frac{1}{u} e^{-ut} \sin\left[(u-a_1)^{1/2} x\right] \times$$

$$[1-e^{ut_o} H(t-t_o)]\, du\}. \qquad (9.26)$$

where

$$a_1 = \frac{U^2}{4} + k.$$

(iii) When the flux is step function i.e. $W(t) = W_o \quad 0 < t \leq t_o$

$$= 0 \qquad t > t_o$$

$$C(x,0,0,t) = \frac{P(x)}{4\pi x}\{\exp\left[-\left(\frac{U^2}{4} + \frac{\alpha_1}{\alpha}\right)^{1/2} x\right](1-H(t-t_o))$$

$$- \frac{1}{\pi}\int_a^{\alpha} \frac{1}{u}\left[1-e^{ut_o}H(t-t_o)\right]M(x,u,t)\,du$$

$$- \frac{1}{\pi}\int_{a'}^{\infty} \frac{1}{u}\left[1-e^{ut_o}H(t-t_o)\right]M(x,u,t)\,du\} \qquad (9.25)$$

Where $H(t-t_o)$ is defined by (Carslaw and Jaegar, 1941)

$$H(t-t_o) = 0 \qquad t \leq t_o$$

$$= \frac{t}{t_o+\epsilon} \qquad t_o < t \leq t_o + \epsilon$$

$$= 1 \qquad t > t_o.$$

In this case, for instantaneous removal the concentration distribution along the central line, in the diemsnsicnless form, is given by

$$C_1(x,0,0,t) = \frac{P(x)}{4\pi x}\{\exp\left[-\left(\frac{U^2}{4} + k\right)^{1/2} x\right] \times$$

$$\left[1-H(t-t_o)\right] - \frac{1}{\pi}\int_{a_1}^{\infty} \frac{1}{u} e^{-ut} \sin\left[(u-a_1)^{1/2} x\right] \times$$

$$\left[1-e^{ut_o}H(t-t_o)\right]\,du\}. \qquad (9.26)$$

Now to compare the case of delayed removal with instantaneous removal we consider the following cases

(i) $k > \frac{\alpha_1}{\alpha}$ (ii) $k = \frac{\alpha_1}{\alpha}$ (iii) $k < \frac{\alpha_1}{\alpha}$

For $k > \frac{\alpha_1}{\alpha}$, it is observed that for all the three types of sources, the concentration of pollutant for the case of delayed removal is greater than in the case of instantaneous removal (see figs. 9.1, 9.4, 9.7). In the case of constant flux, it is noted that even if $k \leq \frac{\alpha_1}{\alpha}$, the concentration of the pollutant for the case of delayed removal is always greater than instantaneous removal case (see figs. (9.4-9.6)). However, for other two typesof sources when $k \leq \frac{\alpha_1}{\alpha}$, the concentration in the delayed removal case can be less, equal, or greater than the instantaneous removal case and this behaviour depends upon the downwind distance from the source, time elapsed, etc. (see figs. 9.2-9.3, 9.8-9.9). The results can be visualized by comparing the removal mechanism in equations (9.1), (9.5) and noting that the integrand in the integral term in equation (9.5) involves a negative exponential which decreases as t or α increases.

To observe the effect of wind velocity on the concentration of air pollutant at different locations and times, see figs. 9.10-9.12. It is noted from fig. 9.10 that, for instantaneous flux, the concentration of pollutant at a fixed instant increases at different locations and the point

of maximum in the concentration distance profile moves away from the source as wind velocity increases. For constant flux, (see fig. 9.11) the concentration increases as wind velocity increases at a particular time and location. However, when the flux is given by step function, (see fig. 9.12) the concentration increases as wind velocity increases for fixed $t \leq t_o$, but when $t > t_o$, the increase or decrease in concentration with respect to wind velocity depends upon downwind distance from the source.

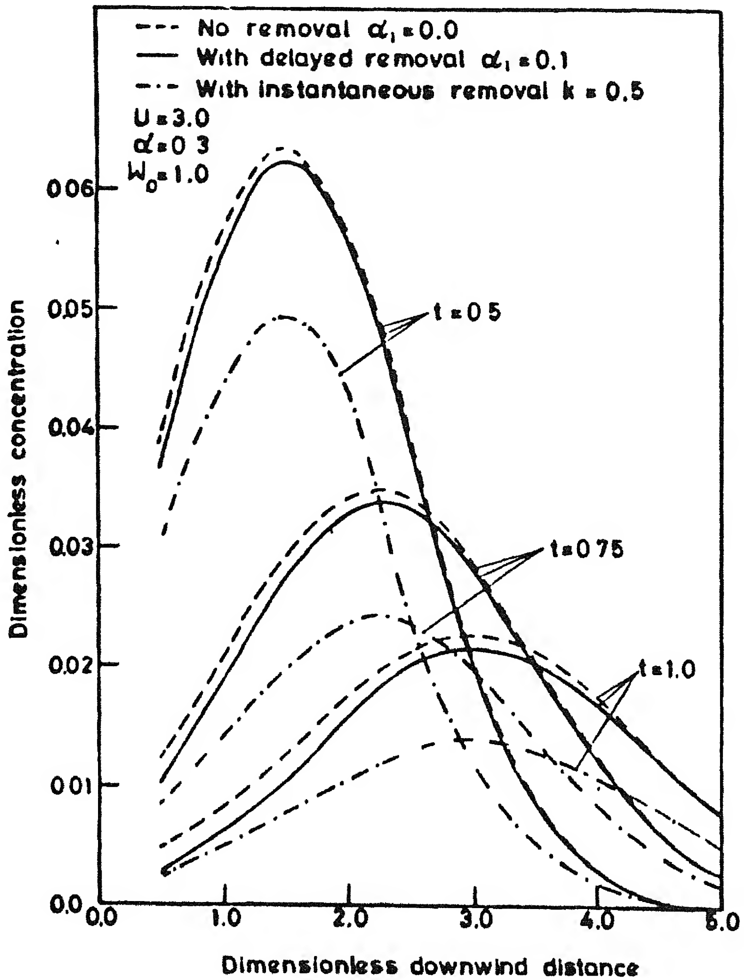

FIG NO 9.1 FLUX IS INSTANTANEOUS AT THE SOURCE

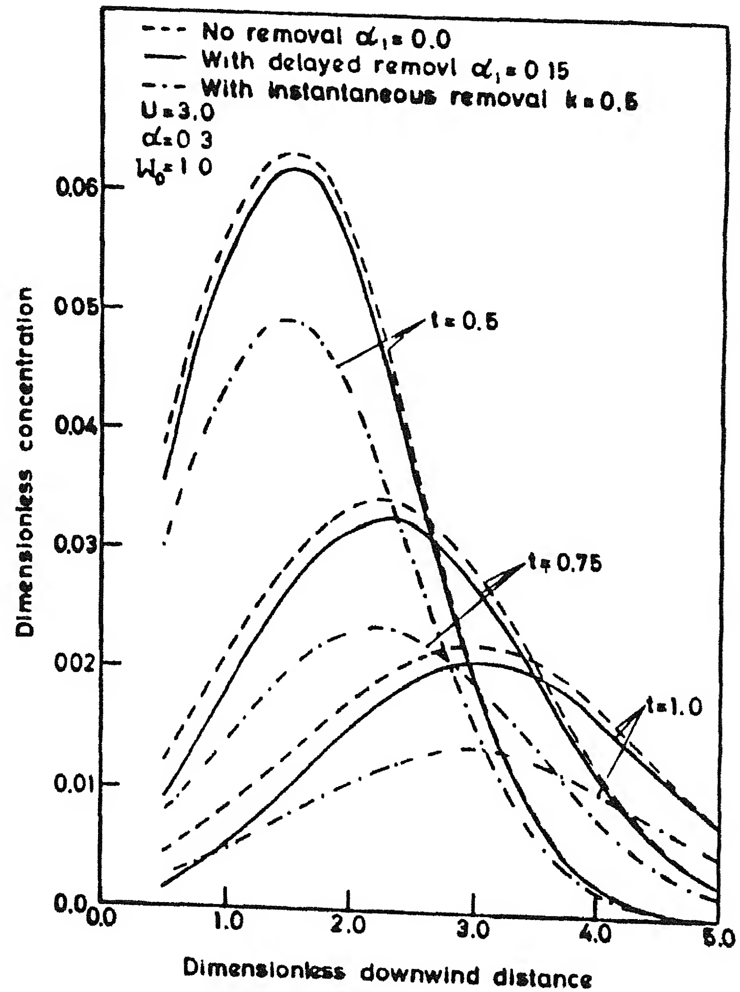

FIG NO 9.2 FLUX IS INSTANTANEOUS AT THE SOURCE

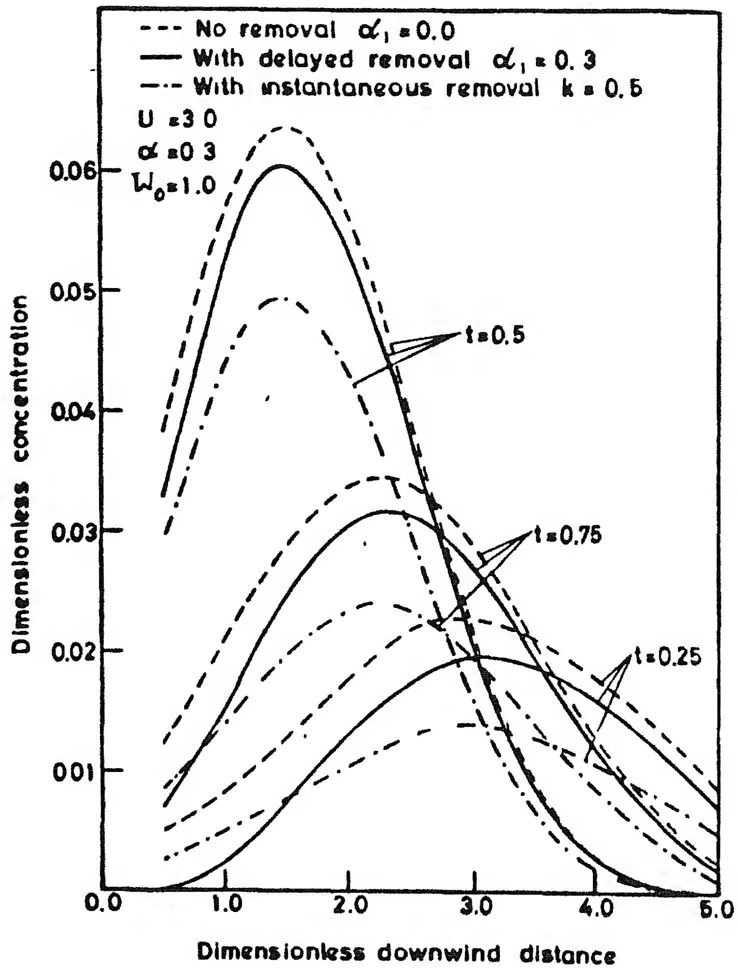

FIG NO 9 3 FLUX IS INSTANTANEOUS AT THE SOURCE

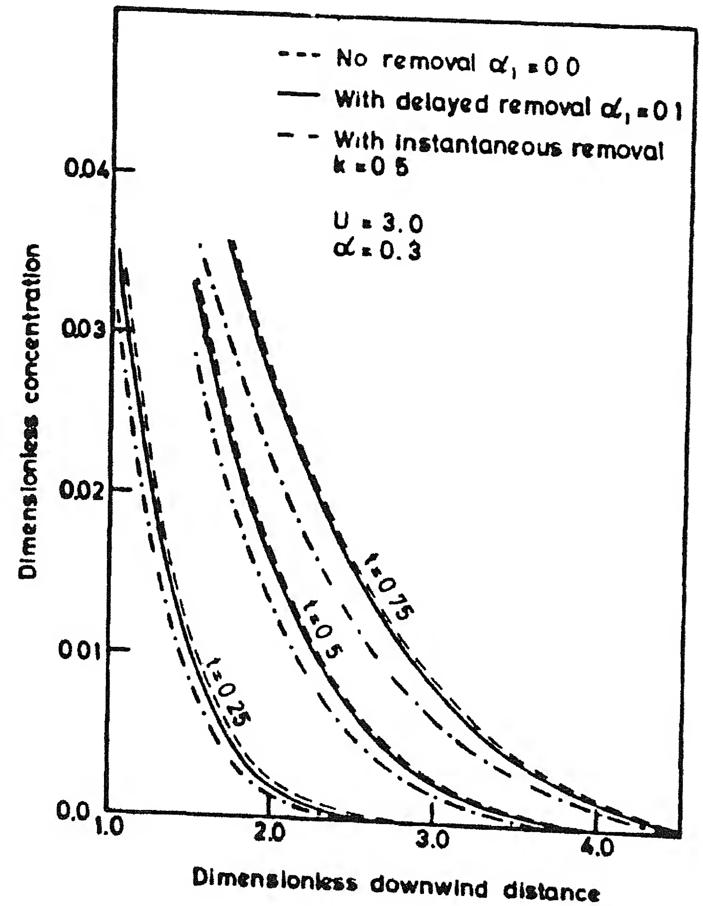

FIG NO 9 4 FLUX IS CONSTANT AT THE SOURCE

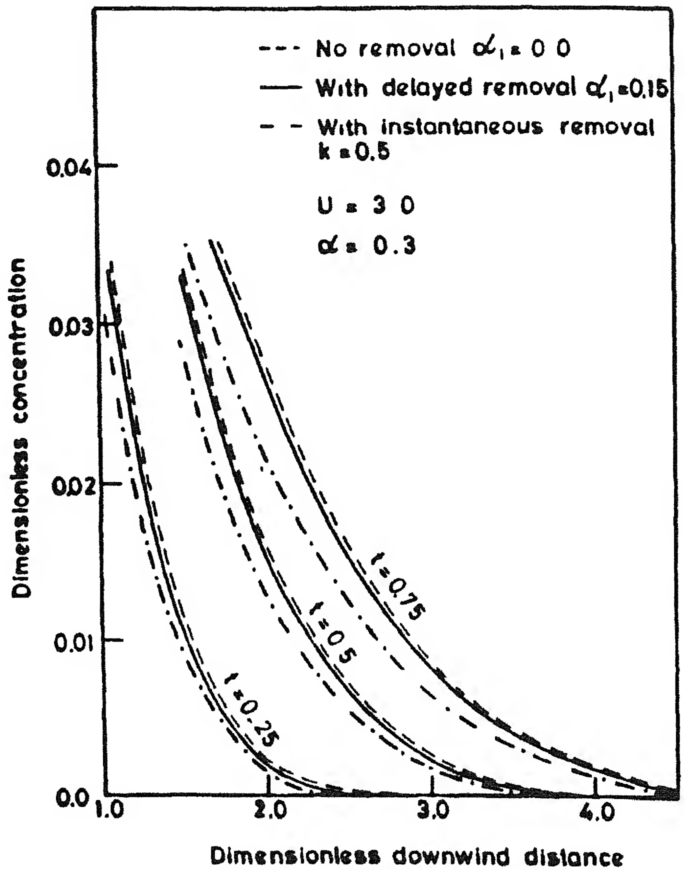

FIG NO 9.5 FLUX IS CONSTANT AT THE SOURCE

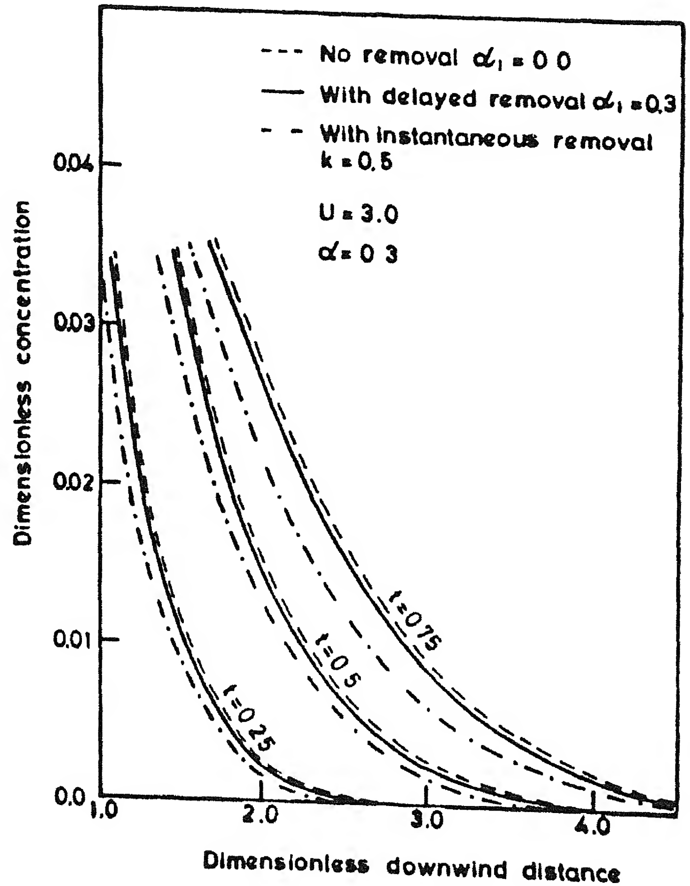

FIG NO 9.6 FLUX IS CONSTANT AT THE SOURCE

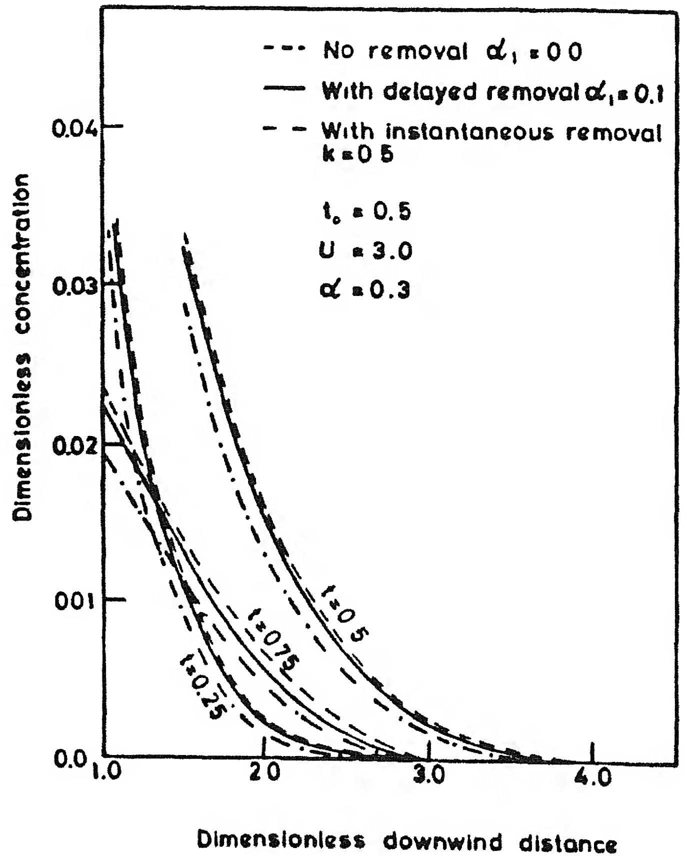

FIG NO 9.7 FLUX IS STEP FUNCTION TYPE AT THE SOURCE

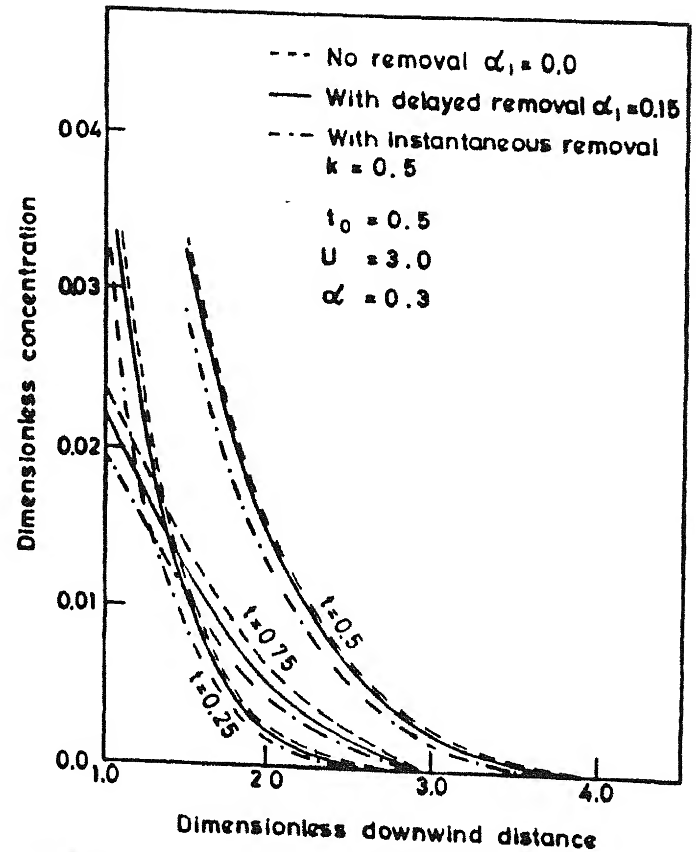

FIG NO 9.8 FLUX IS STEP FUNCTION TYPE AT THE SOURCE

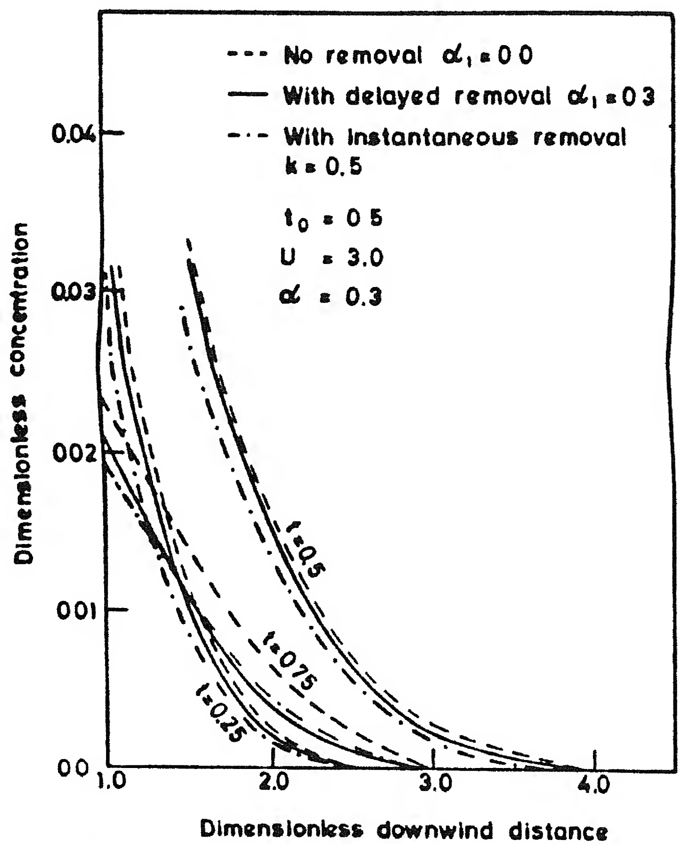

FIG NO 9.9 FLUX IS STEP FUNCTION TYPE AT THE SOURCE

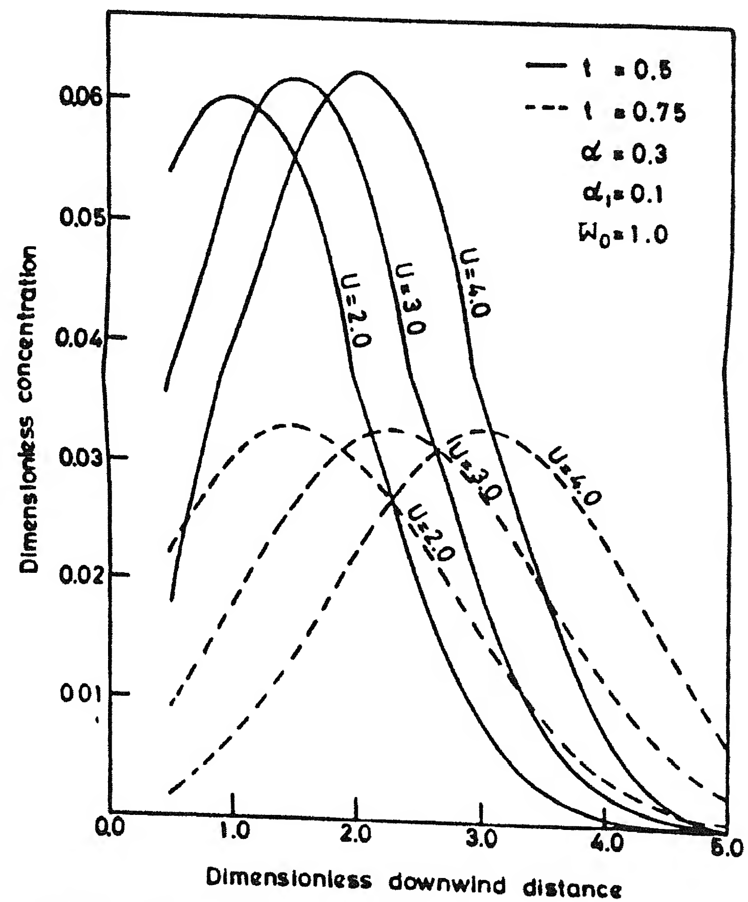

FIG NO 9.10 FLUX IS INSTANTANEOUS AT THE SOURCE

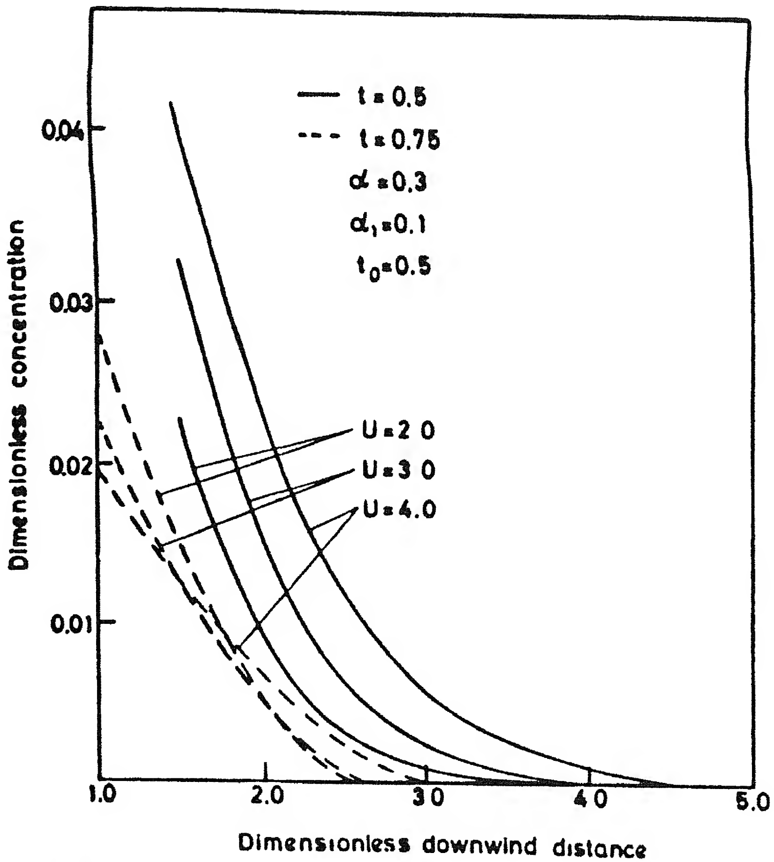

FIG NO 9.12 FLUX IS STEP FUNCTION TYPE AT THE SOURCE

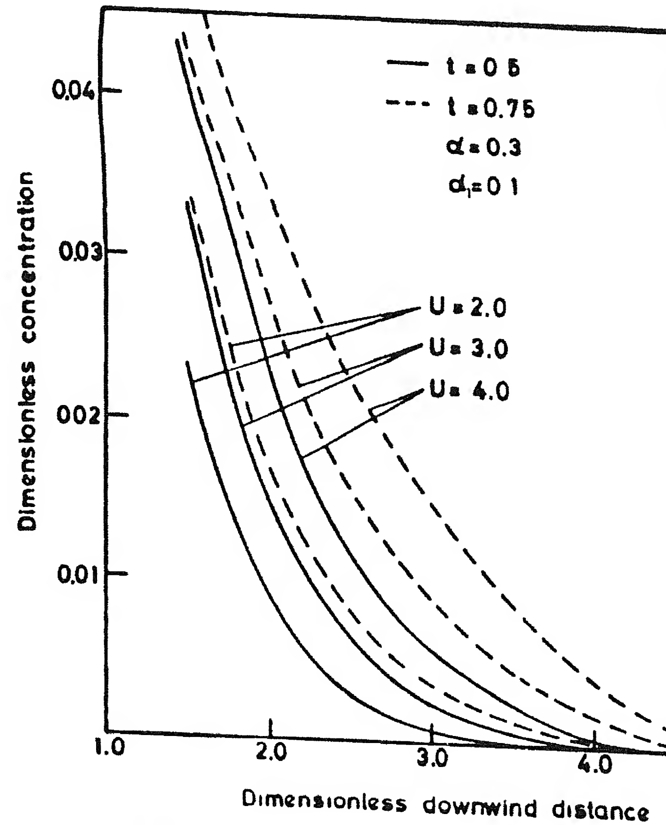

FIG NO 9 11 FLUX IS CONSTANT AT THE SOURCE

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